

Hydrogenative Depolymerization of Nylons

Authors: Amit Kumar^{1δ}, Niklas von Wolff², Michael Rauch¹, You-Quan Zou^{1‡}, Guy Shmul³, Yehoshua Ben-David³, Gregory Leitus³, Liat Avram³, David Milstein^{1*}

Affiliations:

¹Department of Organic Chemistry, ³Department of Chemical Research Support, The Weizmann Institute of Science, Rehovot 76100, Israel. ²Laboratoire d'Electrochimie Moléculaire, UMR 7591, CNRS/University of Paris, 75013 Paris, France. Current address: ^δSchool of Chemistry, University of St. Andrews, KY169ST, UK; [‡]Department of Chemistry, University of Cambridge, CB21EW, UK.

*Correspondence to: david.milstein@weizmann.ac.il

Table of Contents

1.	Materials and methods	S3-S4
2.	General procedure for the catalytic hydrogenation of nylons	S4-S6
3.	Optimization table for the catalytic hydrogenative depolymerization of nylon 6	S6-S10
4.	NMR Spectral data for the hydrogenative depolymerization of nylon 6	S10-S15
5.	GC data for the hydrogenative depolymerization of nylon 6	S16
6.	ESI-MS data for the hydrogenative depolymerization of nylon 6	S17
7.	Separation of products (6-amino-1-hexanol and the oligomers) by LC-MS and determination of estimated yields	S17-S21
8.	Estimation of the size of oligomers using DOSY NMR spectroscopy	S21-S22
9.	Sequential hydrogenation of nylon 6	S21-S24
10.	Isolation of 6-amino-1-hexanol after the hydrogenation of nylon-6 in DMSO	S25-S28
11.	Measurement of the molecular weight of the nylons (polyamides)	S28-S30
12.	Spectral details of the catalytic hydrogenation of other polyamides	S30-S39
13.	Demonstration of the closed loop cycle	S40-S42
14.	Mechanistic studies	S43-S61
15.	Crystallographic details	S61-S63
16.	DFT calculations	S63-S67
17.	References	S67-S69
18.	Energies and cartesian coordinates of computed structures	S70-S138

1. Materials and Methods

All experiments were carried out in M-BRAUN Unilab 1200/780 glovebox under inert atmosphere of purified nitrogen or using standard Schlenk techniques. THF, 1,4-dioxane, toluene and *n*-pentane were refluxed over sodium/benzophenone, distilled under argon atmosphere, and stored over 4 Å molecular sieves (MS). DMSO (assay > 99.7%, not dry) was purchased from Holland Moran and used as received. Diglyme, meta cresol, DMF, anisole and HMPA (Hexamethylene phospharamide) were purchased from Holland Moran or Sigma-Aldrich and used as received. Nylon 6 (resins, size 3 mm, Mw = 10,000) was purchased from Sigma-Aldrich and used as received. Nylon 6 (powder) was purchased from the Goodfellow and used as received. Nylon 12 was purchased from Sigma-Aldrich and used as received. Other polyamides shown in Table 2 of the manuscript were prepared using the method reported by us earlier.¹ Ruthenium complexes **1-2**,² **3**,³ **4**,⁴ **5**,⁵ **6**,⁶ and **7**,⁷ were synthesized according to the methods reported earlier in the literature. The dimer, 6-amino-N-(6-hydroxyhexyl)hexanamide (**O2**) was synthesized as per the procedure reported in literature.⁸ Deuterated solvents were degassed with argon and kept in the glovebox over 4 Å MS. KO*t*Bu (sublimed grade, 99.99%) was purchased from the Sigma-Aldrich and used as received. ¹H NMR, ¹³C{¹H} NMR, and ³¹P{¹H} NMR spectra were recorded on a Bruker Avance III HD-500 and Avance III-400 NMR spectrometer and reported in ppm (δ). ¹H NMR and ¹³C{¹H} NMR chemical shifts are referenced with respect to tetramethylsilane, while ³¹P{¹H} NMR chemical shifts are reported referenced to an external 85% solution of phosphoric acid in H₂O.

Details for the ESI-MS Experiments:

The analyses were carried out on a Waters Xevo G2-XS QTof mass spectrometer (Manchester, UK) with an electrospray ionisation (ESI) source operating in the positive mode. The samples were directly infused at a flow rate of 10 μ L/min. All spectra were acquired in the mass range of 50–2000 m/z. The positive matches were limited with mass error of not more than 5.0 ppm.

The following settings were applied: a capillary voltage of 1.0 kV, cone gas flow was 28 L/h, source temperature was set at 120 °C and the cone voltage was set at 40 V. The desolvation temperature was set at 350 °C and the desolvation gas (N_2) flow rate was set at 550 L/h. All measurements were done using Leucine-Enkephalin (200 μ g/uL, acetonitrile:H₂O containing 0.1% formic acid (1:1, v/v)) as a lockspray reference at flow rate of 10 uL/min to ensure mass accuracy and follow resolution mode. Data acquisition and recording was done by Waters MassLynx v4.2 software.

Details for the GC experimental setup and the method used:

GC system: HP 6890 or Agilent 7890B Series.

Column: HP-5 5% Phenyl methyl siloxane, 30 m, 320 μ m.

Inlets: 280 °C, Detector: FID 280 °C; Carrier Gas: He. Flow: 1 mL/min.

Oven: 130 °C, hold 4 min; 15 °C/min to 280 °C, hold 18 min.

2. General procedure for the catalytic hydrogenation of nylons

Complex **1** (10 mg, ~0.02 mmol) and KO^tBu (9 mg, 0.08 mmol) were dissolved in the given solvent (2.5 mL) to which resins of nylon 6 (~117 mg, 1 mmol relative to the monomer) was added. The reaction mixture was transferred to an autoclave and pressurized with H₂ (60-70 bars). The autoclave was heated at 135-150 °C under continuous stirring for 48-72 h depending on the conditions described in tables below. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood. Mesitylene (120 mg, 1 mmol) was added to the reaction mixture as an internal standard and the reaction mixture was analyzed by GC, GC-MS, ESI-MS and ¹H NMR spectroscopy. The yield of 6-amino-1-hexanol was determined by GC using mesitylene as an internal standard.

Method for determining conversion of the depolymerization of nylon 6:

The conversion of nylon 6 was determined by measuring the weights of the solid reaction mixture before and after the reaction, based on the observation* that nylon 6 has no solubility in DMSO at room temperature. After completion of the reaction, GC of the crude reaction mixture was recorded to get the yields of 6-amino-1-

hexanol. The reaction mixture was then filtered, collecting all the insoluble, unreacted nylon 6, followed by removal of the DMSO and the internal standard (mesitylene) under vacuum at 80-100 °C. The weight of the obtained materials contained only hydrogenated nylons and catalysts. Based on the weight of the residual materials and knowing the weight of the starting materials without solvents, we can calculate the conversion of nylons by weight.

An example for the calculation is illustrated here for Table S1, entry 6.

Weight of starting mixture before hydrogenation [nylon (117 mg) +Ru-complex (10 mg) +base (9 mg)] = 136 mg.

Weight of the insoluble solids after hydrogenation = 97 mg

Weight of material originating from nylon = 78 mg (97-19)

Maximum weight originating from nylon after hydrogenation = 121 mg (2 eq of hydrogen each monomer)

Conversion of nylon = 65%

The evacuated residue was dissolved in CDCl_3 , filtered and characterized by NMR spectroscopy and ESI-Mass spectrometry.

*To verify that the unreacted nylon 6 is insoluble in DMSO, 117 mg of nylon 6 (resins) was heated in DMSO (4 mL) at 150 °C for 6 h in a pre-weighed Young's Schlenk tube, resulting in a clear homogenous solution, which was allowed to cool down to room temperature. At room temperature, formation of a white precipitate was observed. Some DMSO was pipetted out from the mixture and the remaining DMSO was removed at 80-100°C under pressure 10^{-2} atm. ~116 mg of solid was obtained after the distillation indicating that at room temperature the nylon 6 which had dissolved in DMSO at 150°C, quantitatively precipitated at room temperature.

Molecular weight of the recovered nylon 6 after hydrogenation (filtering from the dmso solution) was also calculated by the end group analysis using ^1H NMR spectroscopy (in d-TFA) which showed it to be \sim 9400 (Fig S1A), slightly lower than that of the starting nylon 6 (\sim 10,000).

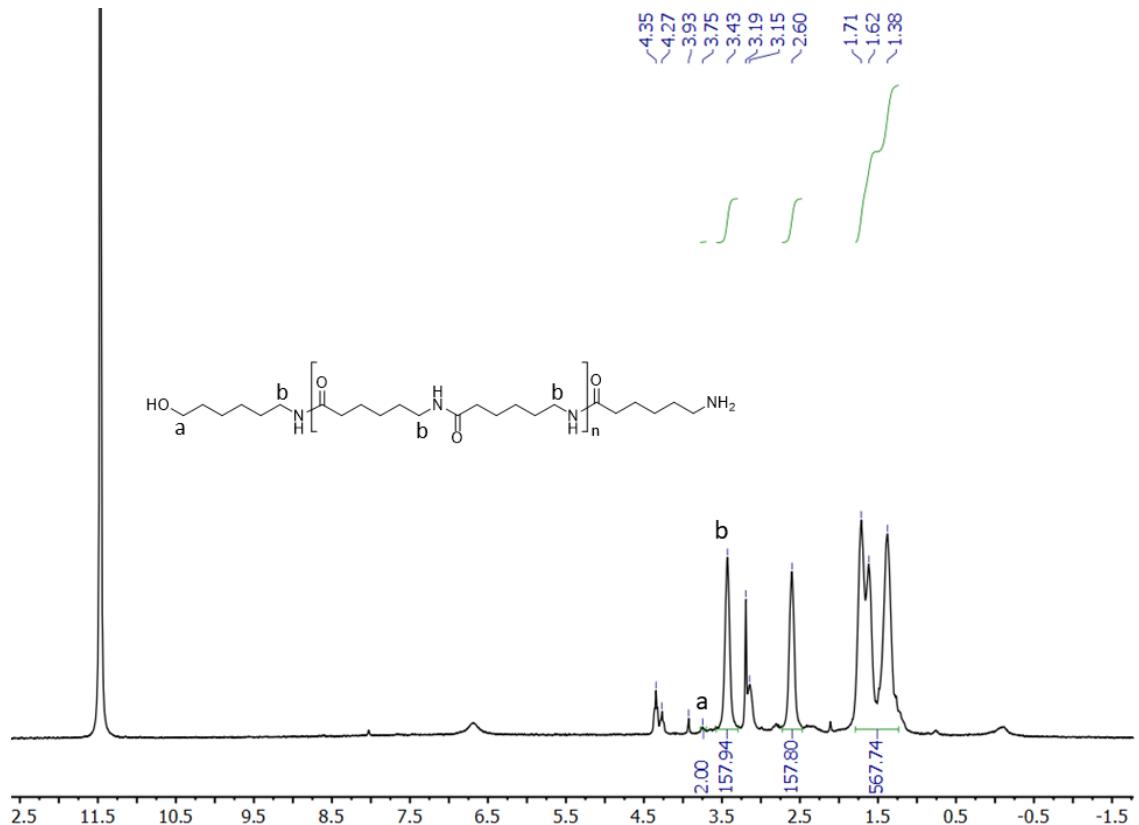


Figure S1A. ^1H NMR (300MHz, 298K, d-TFA) spectrum of the recovered nylon 6 after hydrogenation.

3. Optimization tables for the catalytic hydrogenative depolymerization of nylon 6

3.1. Solvent screening:

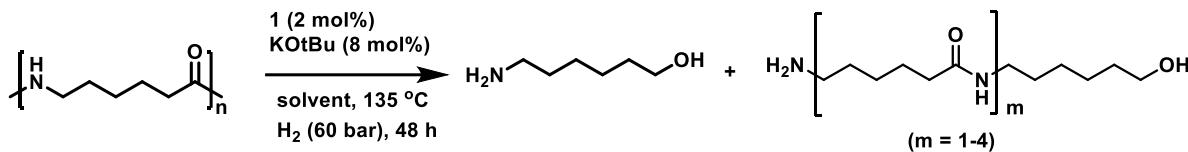


Table S1. Solvent screening for the catalytic hydrogenative depolymerization of nylon 6.^a

entry	solvent	conversion	Yield of amino alcohol	Oligoamide detection	remark
1.	Toluene	0%	Not detected	no	Resins recovered
2.	THF	0%	Not detected	no	Resins recovered
3.	1,4-Dioxane	0%	Not detected	no	Resins recovered
4.	Water	0%	Not detected	no	Resins recovered
5.	DMF	0%	Not detected	no	Resins recovered
6.	DMSO	65%	14%	yes	No resins recovered
7.	Anisole	10%	Not detected	yes	Resins recovered (broken)
8.	Hexamethylene phospharamide	30%	Not detected	yes	Resins recovered (broken)
9.	BMIM-OctSO ₄	0%	Not detected	no	Resins recovered
10.	Diglyme	30%	0.2%	yes	Resins recovered (broken)
11.	Meta-cresol	50%	5%	yes	No resins recovered
12.	Dioxane/DMSO (4:1)	20%	Not detected	yes	Resins recovered (broken)
13.	Dioxane/m-cresol (4:1)	30%	1%	yes	Resins recovered (broken)
14.	Anisole/DMSO (4:1)	10%	Not detected	yes	Resins recovered (broken)

^aCatalytic conditions: Nylon 6 (117 mg, 1 mmol relative to the mol wt of the monomer), complex 1 (10 mg, 0.02 mmol), KO^tBu (9 mg, 0.08 mmol), solvent (2.5 mL), temperature 135 °C and reaction time 48 h. “Resins recovered” means complete recovery of resins with the shape and size intact. “Resins recovered (broken)” means that the resins were broken to small pieces after the reaction.

3.2. Variation of pressure, catalytic loading, temperature and reaction time

Table S2. Variation of pressure, catalytic loading, temperature and reaction time^a

Entry	complex (mol%)	Base (mol%)	time	temp	H ₂ (bar)	Amino-alcohol (yield%)	conversion
1	1 (2 mol%)	KOtBu (8 mol%)	48 h	135 °C	60 bar	14%	65%
2	1 (2 mol%)	KOtBu (8 mol%)	48 h	150 °C	60 bar	19%	70%
3	1 (2 mol%)	KOtBu (8 mol%)	48 h	135 °C	70 bar	18%	75%
4	1 (2 mol%)	KOtBu (8 mol%)	48 h	150 °C	70 bar	24%	75%
5	1 (2 mol%)	KOtBu (8 mol%)	72 h	150 °C	70 bar	25%	77%
6	1 (2 mol%)	KOtBu (8 mol%)	24 h	150 °C	70 bar	15%	40%
7	1 (2 mol%)	KOtBu (8 mol%)	144 h	150 °C	70 bar	25%	81%
8	1 (2 mol%)	KOtBu (8 mol%)	48 h	175 °C	70 bar	Not detected	22%
9	1 (5 mol%)	KOtBu (20 mol%)	72 h	150 °C	70 bar	35%	88%

^aCatalytic conditions: Nylon 6 (117 mg, 1 mmol relative to the mol wt of the monomer), complex **1** (10 mg, 0.02 mmol), KOtBu (9 mg, 0.08 mmol), DMSO (2.5 mL), temperature 135 °C - 175 °C, reaction time 48 -72 h and H₂ (60-70 bars) as specified.

3.3. Variation of additives

Complex **1** (10 mg, ~0.02 mmol) and KOtBu (9 mg, 0.08 mmol) were dissolved in DMSO (2.5 mL) to which resins of nylon 6 (~117 mg, 1 mmol relative to the monomer) and the additive were added as described in Table S3. The reaction mixture was transferred to an autoclave and pressurized with H₂ (70 bars) and heated at 150 °C under continuous stirring for 48 h. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood. Mesitylene (120 mg, 1 mmol) was added to

the reaction mixture as an internal standard and the reaction mixture was analysed by GC, ESI-MS and ^1H NMR spectroscopy.

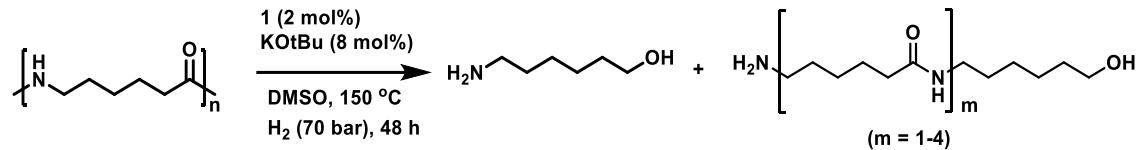


Table S3. Variation of additives^a

Entry	additive	conversion	Amino-alcohol (yield%)	Oligoamide detection	remark
1	Mol-sieves	70%	18%	yes	No resins recovered
2	Water (20 mol% wrt nylon)	30%	Not detected	yes	Resins recovered (broken)
3	LiCl (5% by wt wrt the DMSO)	25%	Not detected	yes	Resins recovered (broken)
4	Sc(OTf) ₃ (1 % by wt wrt the DMSO)	30%	Not detected	yes	Resins recovered (broken)

^aCatalytic conditions: Nylon 6 (117 mg, 1 mmol relative to the mol wt of the monomer), complex 1 (10 mg, 0.02 mmol), KO^tBu (9 mg, 0.08 mmol), DMSO (2.5 mL), temperature 150 °C, reaction time 48 h and H₂ (70 bars). “Resins recovered (broken)” means that the resins were broken to small pieces after reaction.

3.4. Variation of catalysts

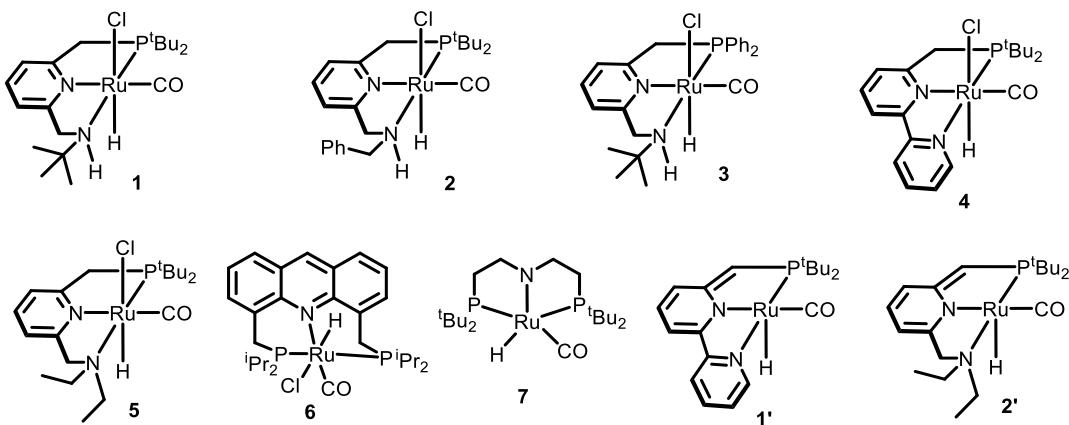


Table S4. Variation of catalysts^a

Entry	complex (2 mol%)	KOtBu	Amino-alcohol (yield%)	conversion	Oligoamide detection	remark
1	1	8 mol%	24%	77%	yes	No resins recovered
2	1	50 mol%	5 %	20%	yes	Resins recovered (broken)
3	1	2 mol%	11 %	35%	yes	Resins recovered (broken)
4	2	8 mol%	26%	80%	yes	No resins recovered
5	3	8 mol%	16%	66%	yes	No resins recovered
6	4	2 mol%	Not detected	30%	yes	Resins recovered (broken)
7	5	2 mol%	Not detected	22%	yes	Resins recovered (broken)
8	6	2 mol%	Not detected	0%	no	Resins recovered
9	7	0 mol%	Not detected	0%	no	Resins recovered
10	1'	0 mol%	Not detected	22%	yes	Resins recovered (broken)
11	2'	0 mol%	Not detected	18%	yes	Resins recovered (broken)

^aCatalytic conditions: Nylon 6 (117 mg, 1 mmol relative to the mol wt of the monomer), complex (0.02 mmol), KOtBu (2-9 mg, 0.02-0.08 mmol) as specified, DMSO (2.5 mL), temperature 150 °C, reaction time 48 h and H₂ (70 bars). “Resins recovered” means complete recovery of resins with the shape and size intact. “Resins recovered (broken)” means that the resins were broken to small pieces after reaction.

4. NMR Spectral data for the hydrogenative depolymerization of nylon 6

4.1 NMR spectra measured in DMSO/CDCl₃:

An aliquot from the reaction mixture (from the Table S2, Entry 4, DMSO solvent) was dissolved in CDCl₃ and the ¹H NMR spectrum was measured as shown below. As can be seen, the characteristic signals in the ¹H NMR spectrum (Fig. S1) coming from the 6-

amino-1-hexanol fall in the region of the signals originating from DMSO (δ 2.5). In order to detect the characteristic signals, a catalytic experiment was performed in DMSO-d6 under the same conditions as described in Table S2, entry 4 and the ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded (Fig. S2-S3).

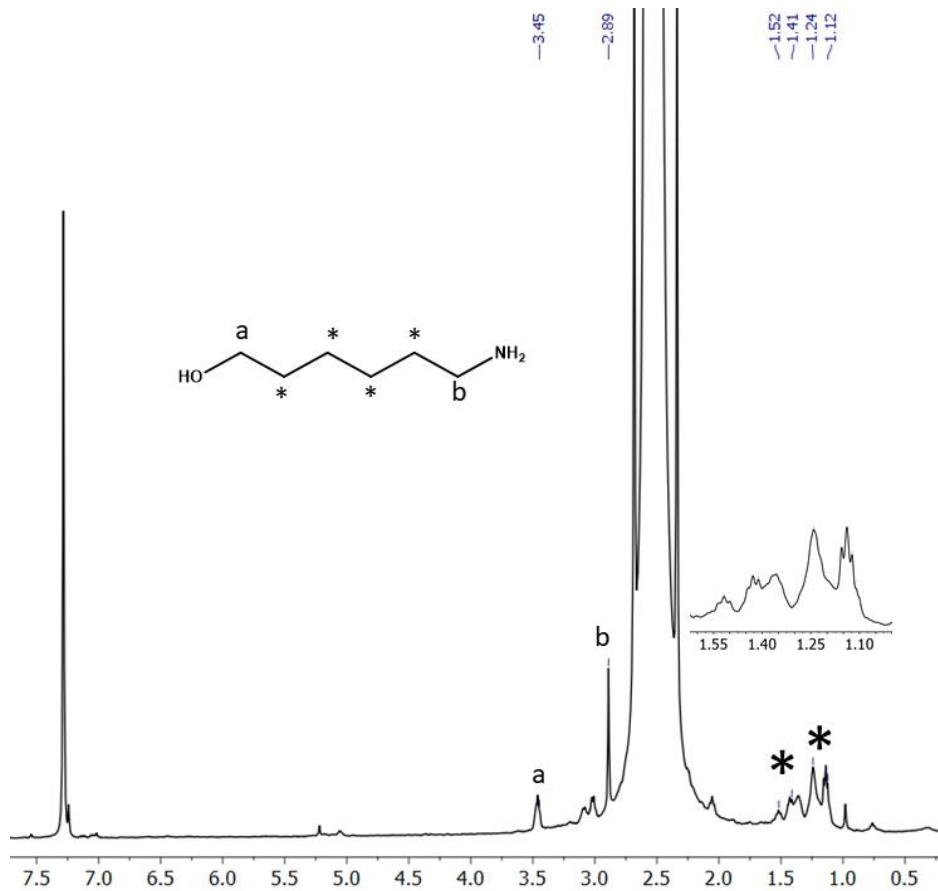


Fig. S1. ^1H NMR (500.08 MHz, 298K, CDCl_3) spectrum of an aliquot from the reaction mixture (Table S2, Entry 4).

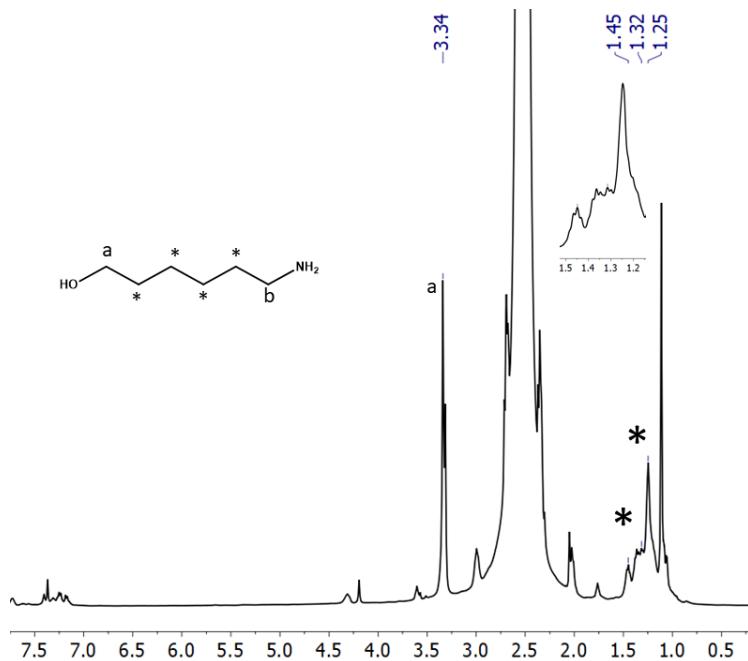


Fig. S2. ^1H NMR (500.08 MHz, 298K, CDCl_3) spectrum of an aliquot from the reaction mixture (Table S2, Entry 4).

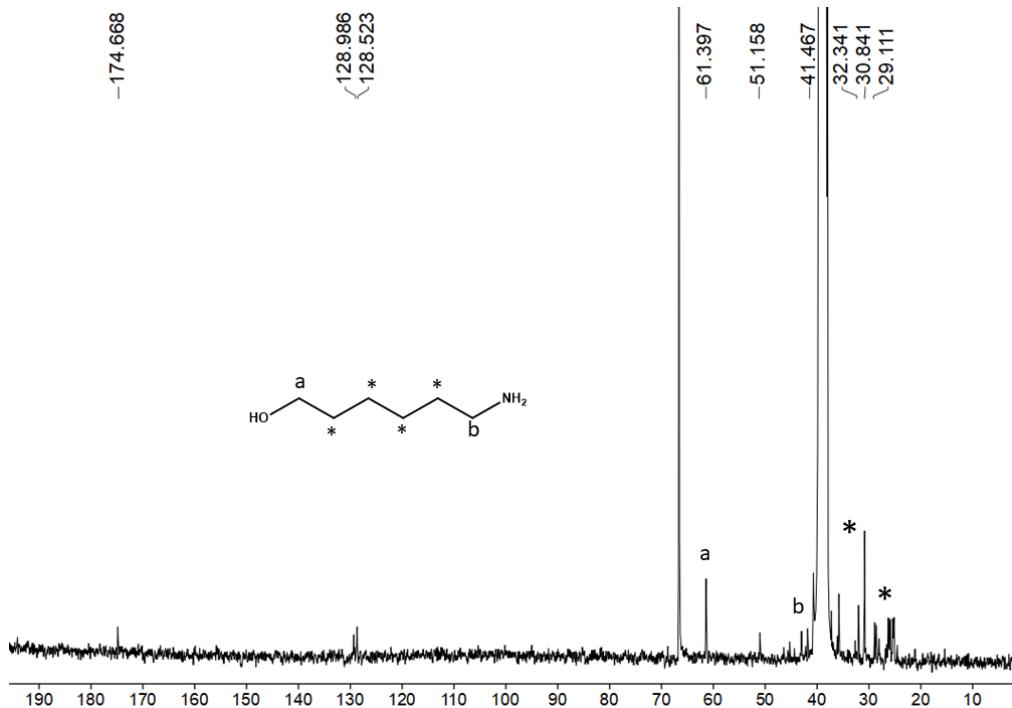


Fig. S3. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298K, CDCl_3) spectrum of the aliquot from the reaction mixture (Table S2, Entry 4). The signal at δ 174.7 is due to the carbonyl carbon of the formed oligoamides.

4.2 NMR spectra measured in CDCl_3 after removal of DMSO

Removal of DMSO:

Removal of DMSO was first attempted by the solvent extraction method. CHCl_3 (5 mL) and H_2O (5 mL) were added to the reaction mixture and the solvent extraction was performed so that the products 6-amino-1-hexanol and oligoamides remain in the CHCl_3 layer whereas DMSO goes in the H_2O layer. However, as 6-amino-1-hexanol is also soluble in H_2O , its yield after extraction in CHCl_3 was reduced as determined by GC. Similarly, the yield of 6-amino-1-hexanol was reduced when DMSO was removed by lyophilization.

DMSO was successfully removed by vacuum distillation at 80 °C (vacuum: in the range of 10^{-2} bar). NMR spectra (Figs. S4-S6) recorded of the distilled DMSO showed purity level of >95%. The residue obtained after removal of DMSO was dissolved in CDCl_3 and its NMR spectra were recorded (Figs. S7-S8).

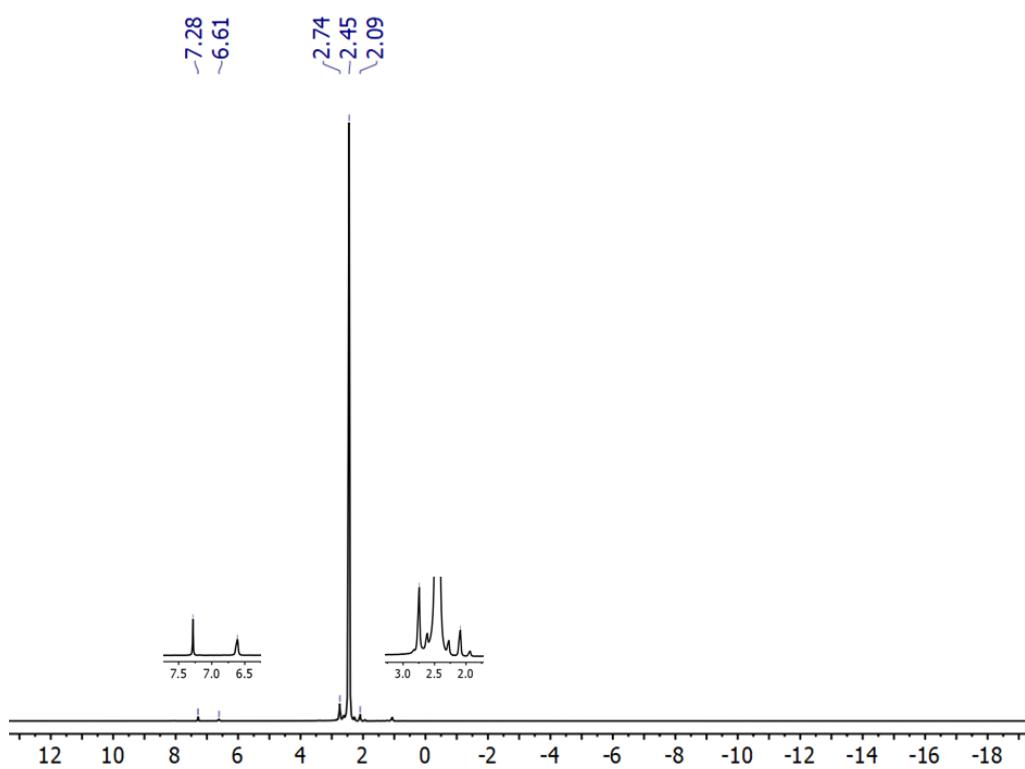


Fig. S4. ^1H NMR (500.08 MHz, 298 K, CDCl_3) spectrum of the distilled DMSO in CDCl_3 after hydrogenation.

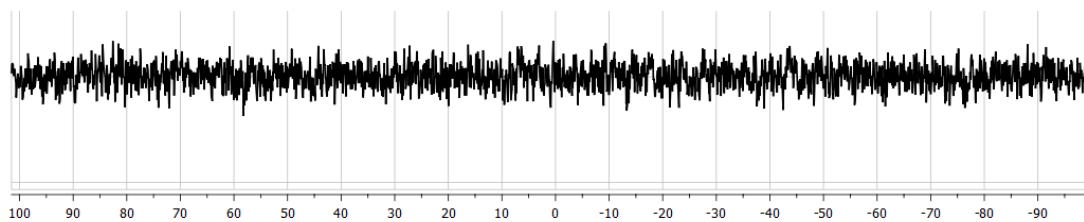


Fig. S5. $^{31}\text{P}\{\text{H}\}$ NMR (202.44 MHz, 298 K, CDCl_3) spectrum of the distilled DMSO in CDCl_3 after hydrogenation.

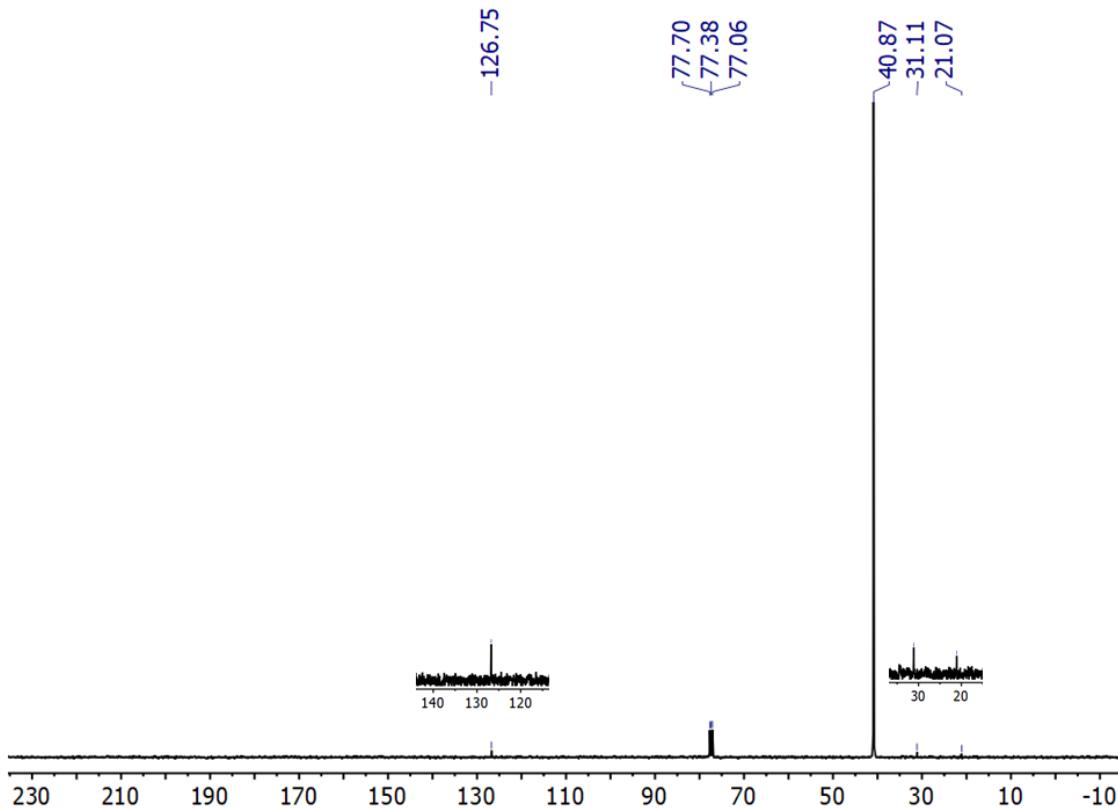


Fig. S6. $^{13}\text{C}\{\text{H}\}$ NMR (500.08 MHz, 298 K, CDCl_3) spectrum of the distilled DMSO in CDCl_3 after hydrogenation.

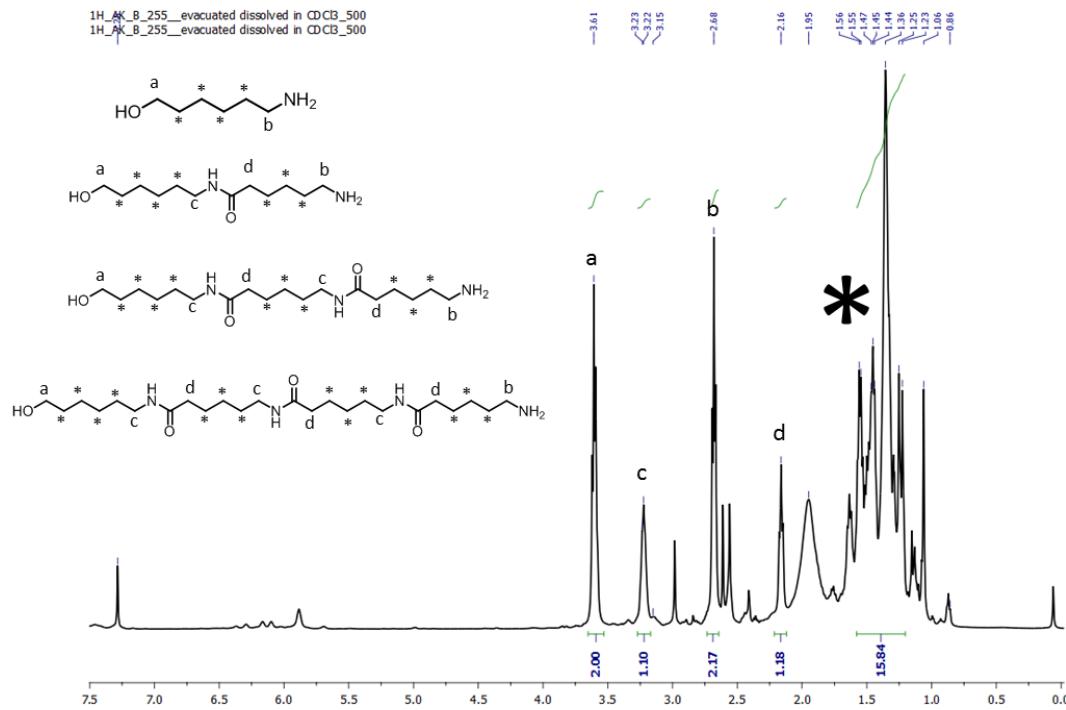


Fig. S7. ¹H NMR (500.08 MHz, 298 K, CDCl₃) spectrum of the reaction mixture in CDCl₃ after removing DMSO.

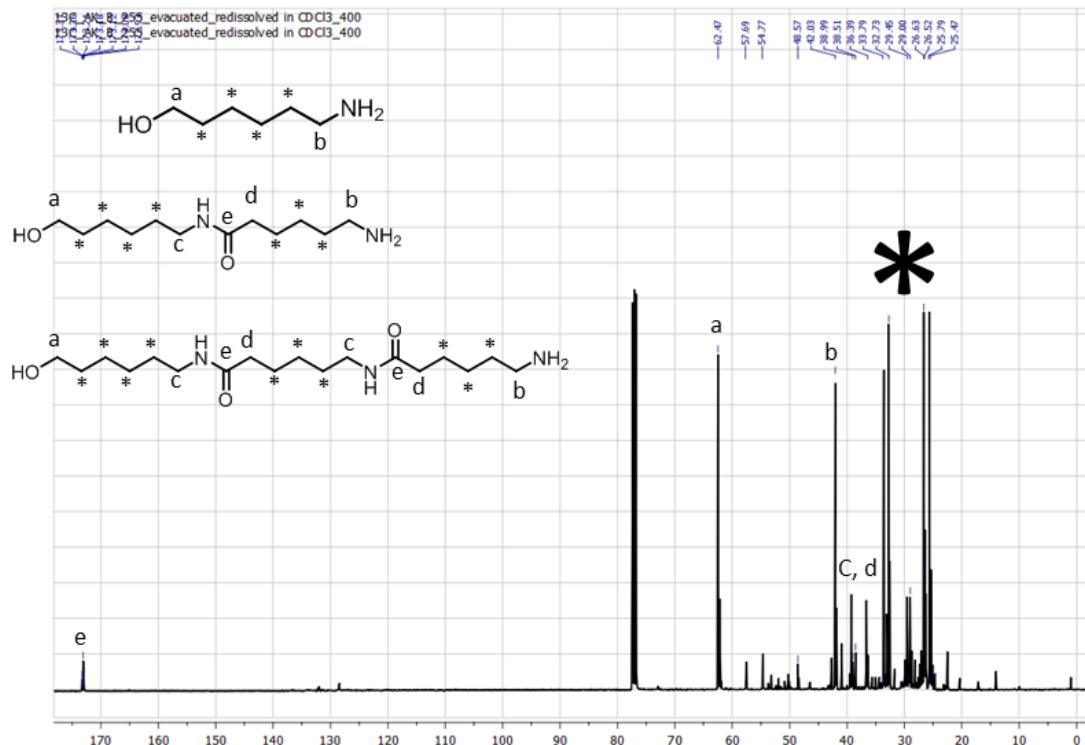


Fig. S8. ¹³C{¹H} NMR (125.75 MHz, 298 K, CDCl₃) spectrum of the reaction mixture in CDCl₃ after removing DMSO.

5. GC data for the hydrogenative depolymerization of nylon 6

After the hydrogenation reaction and the addition of internal standard, the sample in the corresponding solvent (for example DMSO, THF, m-cresol etc. except water) was filtered over celite and directly injected into the GC under the conditions described in the general information section (vide supra). Qualitative calibration of the products (6-amino-1-hexanol (**O1**), caprolactam and the dimer **O2**) was done by injecting them separately under the conditions described above.

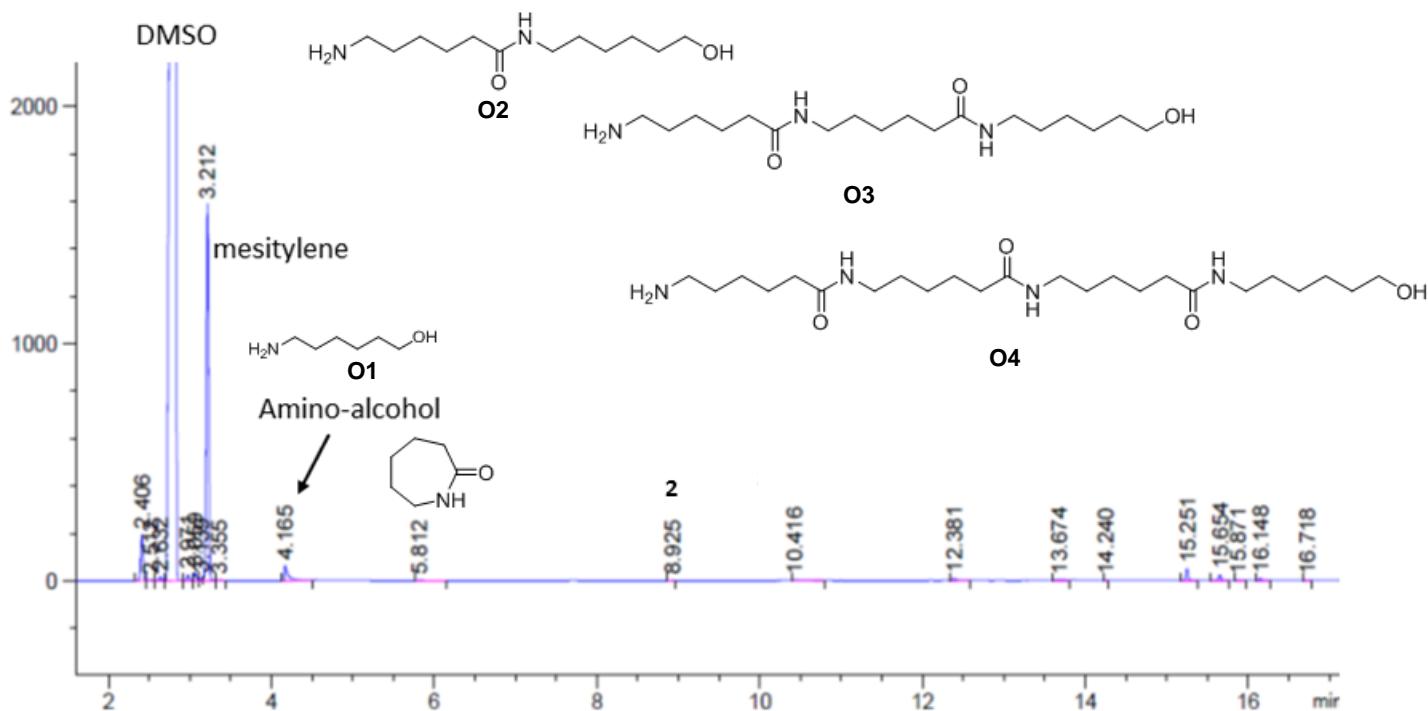


Fig. S9. GC of the reaction mixture after hydrogenation of nylon 6 (Table S2, entry 4). The retention time of 6-amino-1-hexanol, caprolactam and the dimer **O2** were confirmed by injecting their pure samples. The remaining signals are unidentified presumably they are cyclic isomers of trimer and tetramer. Caprolactam is produced only in a trace quantity (<2% yield). We are uncertain about mechanism of its formation. One possibility could be via hydrothermal depolymerisation of nylon 6 or its oligoamides in presence of traces of water present in DMSO. A few examples have been reported for hydrothermal depolymerisation of nylon 6 to caprolactam albeit at higher temperature, for example see: Iwaya et.al. *Polym. Degrad.*, **2006**, 91, 1989-1995 and references therein.

6. ESI-MS data for the hydrogenative depolymerization of nylon 6

DMSO was removed after the hydrogenation step (Table S2, Entry 4) as described above (section 4.2) and the residue was dissolved in CHCl₃ and a HR-ESI-MS spectrum was recorded as per the method described above in the general information section. Analysis of the HR-ESI-MS spectrum obtained in Fig. S10 showed the presence of 6-amino-1-hexanol (**O1**) and oligomers (dimer to tetramer) (**O2-O4** in Fig. S9). The observed masses (m/z) for the 6-amino-1-hexanol and oligomers match well with the corresponding calculated masses (Table S5).

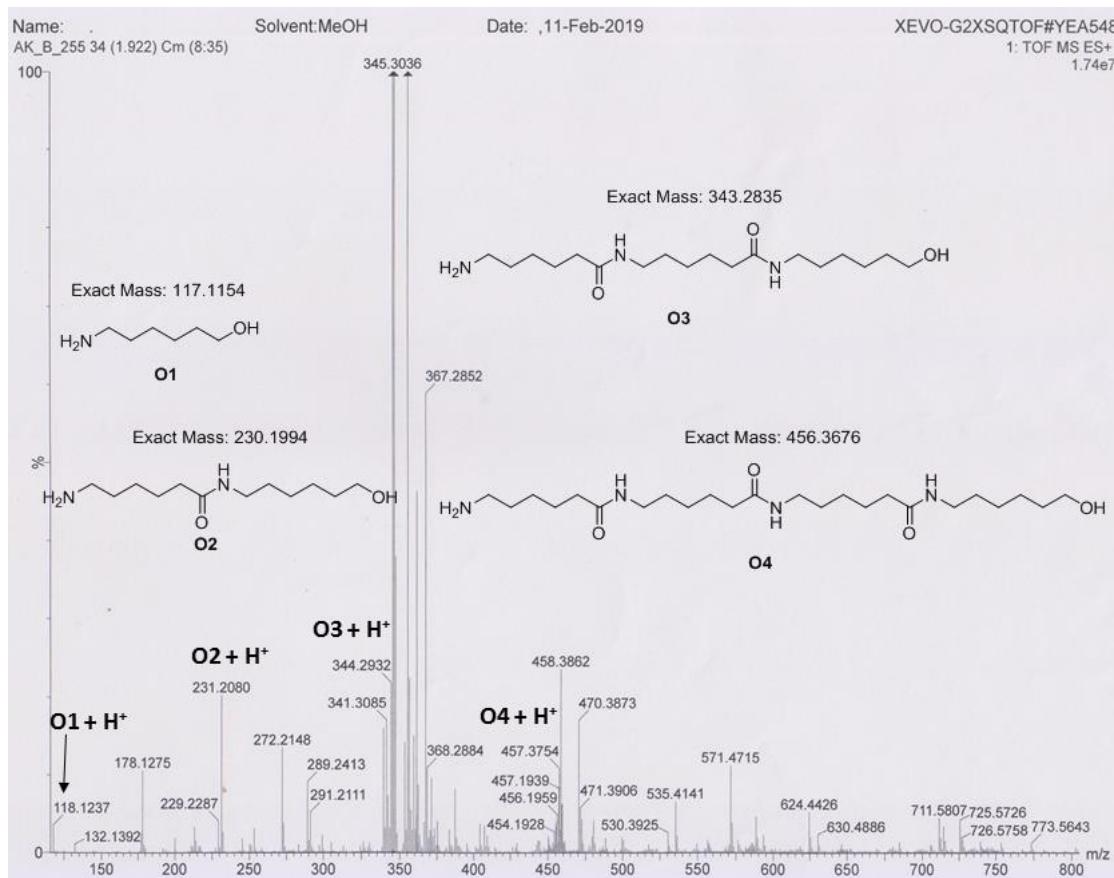
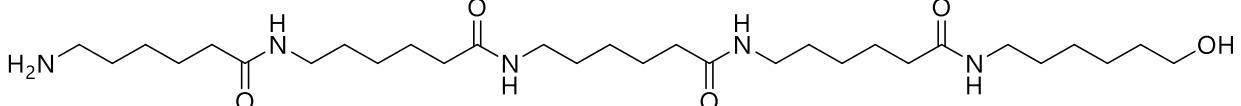


Fig. S10. HR-ESI-MS of the reaction mixture after hydrogenation of nylon-6 (Table S2, entry 4).

7. Separation of products (6-amino-1-hexanol and the oligomers) by the LC-MS and the estimated yields

Table S5. Theoretical and experimental molecular weights of the oligomers obtained after hydrogenation of nylon-6 (Table S2-entry 4).

Peak name	Ion	MS					Mass Error, ppm
		Molecular formula	m/z MH ⁺ ion	Mass, Da			
				Measured	Calculated		
				Chemical Formula: C ₆ H ₁₅ NO Exact Mass: 117.12			
Molecular ion	[M+H] ⁺	C ₆ H ₁₆ NO	118	118.1237	118.1232	4.2	
				Chemical Formula: C ₁₂ H ₂₆ N ₂ O ₂ Exact Mass: 230.20			
Molecular ion	[M+H] ⁺	C ₁₂ H ₂₇ N ₂ O ₂	231	231.2080	231.2073	3.0	
				Chemical Formula: C ₁₈ H ₃₇ N ₃ O ₃ Exact Mass: 343.28			
Molecular ion	[M+H] ⁺	C ₁₈ H ₃₈ N ₃ O ₃	344	344.2928	344.2913	4.4	
				Chemical Formula: C ₂₄ H ₄₈ N ₄ O ₄ Exact Mass: 456.37			

Molecular ion	[M+H] ⁺	C ₂₄ H ₄₉ N ₄ O ₄	457	457.3750	457.3754	0.9
 Chemical Formula: C ₃₀ H ₅₉ N ₅ O ₅ Exact Mass: 569.45						
Molecular ion	[M+H] ⁺	C ₃₀ H ₆₀ N ₅ O ₅	570	570.4612	570.4594	3.2

The chromatographic separation was performed on a Waters Acquity ultra-performance liquid chromatography system, equipped with a quaternary pump system (Milford, MA, USA), using an Acquity BEH C18 column (100 mm × 2.1 mm i.d., 1.7 µm particle size) run at 30 °C. The injection volume was 5 µL. Partial separation was achieved with an isocratic mobile phase at a flow rate of 0.3 mL/min. Solvent A: DDW + 0.1% formic acid; solvent B: acetonitrile+0.1% formic acid. The isocratic elution was: A:B 90:10 (V/V). Detection was done using a Waters SQD2 Mass Detector with an ESCi® source for ESI/APCI switching. The MS detector was operated in the positive mode and the data was acquired in the mass range of 50–2000 m/z. The following mass parameters were applied: cone voltage, 40 V; capillary voltage, 2.80 kV; source temperature, 120 °C; desolvation temperature, 200 °C; cone gas flow rate, 50L/hr; desolvation gas flow rate, 350 L/h. Data acquisition was recorded by MassLynx v 4.2 software.

The separated chromatogram is depicted in Fig. S11. In order to estimate the yields of the hydrogenated products obtained after the hydrogenation of nylon-6 (see Table above), we examined the extracted ion chromatograms for every mass of interest, in order to be able to distinguish between the analyte peaks by inspecting the chromatograms at appropriate m/z values. The results shown here (Fig. S11) are for detection of the compounds of interest and were obtained with 7-point Savitsky-Golay smoothing.

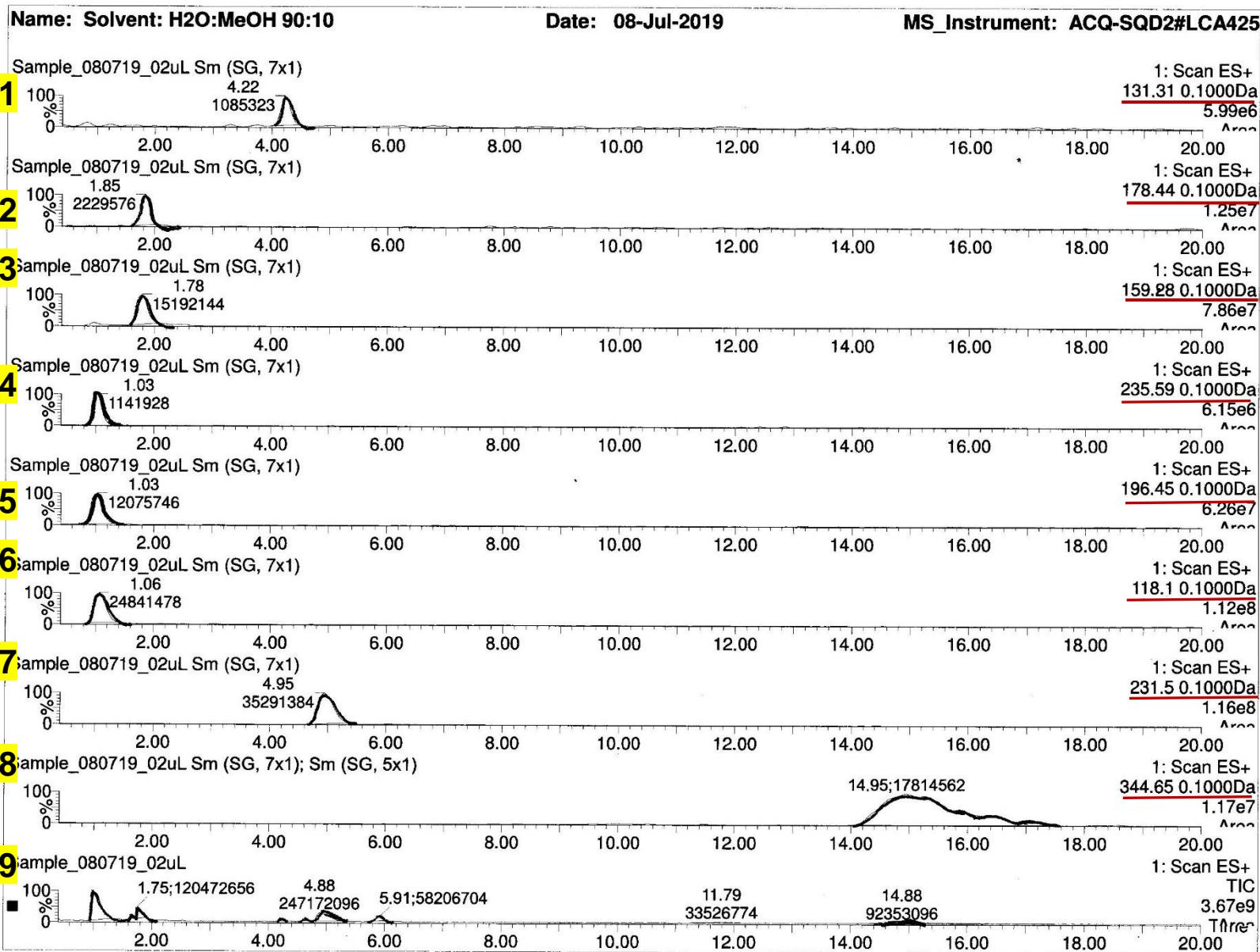


Fig. S11. LC-MS chromatogram of the mixture obtained after the hydrogenation of nylon 6 using the conditions of Table S2, entry 4 (**9**); extraction of chromatogram with m/z = 344.65, trimer (**8**); extraction of chromatogram with m/z = 231.50, dimer (**7**); extraction of chromatogram with m/z = 118.1, amino-alcohol (**6**); extraction of chromatograms whose m/z values have not been identified (**5-1**)

Table S6. Details of the m/z and the corresponding peak areas for the chromatograms that were extracted from the LC-MS run of the hydrogenated nylon 6.

<i>Chromatogram no</i>	<i>m/z</i>	<i>Peak area</i>	<i>% of total</i>	<i>Molecular formula</i>
1	131.3	1085323	1	
2	178.4	2229576	2	
3	159.3	15192144	14	
4	235.6	1141928	1	
5	196.5	12075746	11	
6	118.1	24841478	23	<i>C₆H₁₅NO</i>
7	231.5	35291384	32	<i>C₁₂H₂₆N₂O₂</i>
8	344.7	17814562	16	<i>C₁₈H₃₇N₃O₃</i>
<i>Total</i>		109672141	100	

8. Estimation of the size of oligomers obtained using DOSY NMR spectroscopy

DMSO was removed after the hydrogenation step (Table S2, Entry 4) as described above (section 4.2) and the residue was dissolved in CDCl₃. The resulting solution was analysed by the DOSY NMR spectroscopic technique (500 MHz). The diffusion coefficient corresponding to the oligomers was compared with the diffusion coefficient of 6-amino-1-hexanol (standard sample prepared in CDCl₃ solvent) which showed that the average molecular weight of the oligomers obtained after hydrogenation is 2.8 times that of 6-amino-1-hexanol.

Diffusion coefficient [x10 ⁻⁵ cm ² /s]	7.2ppm	3.6ppm
Monomer	2.35±0.01	1.20±0.01
Mixture	2.35±0.01	0.72±0.01

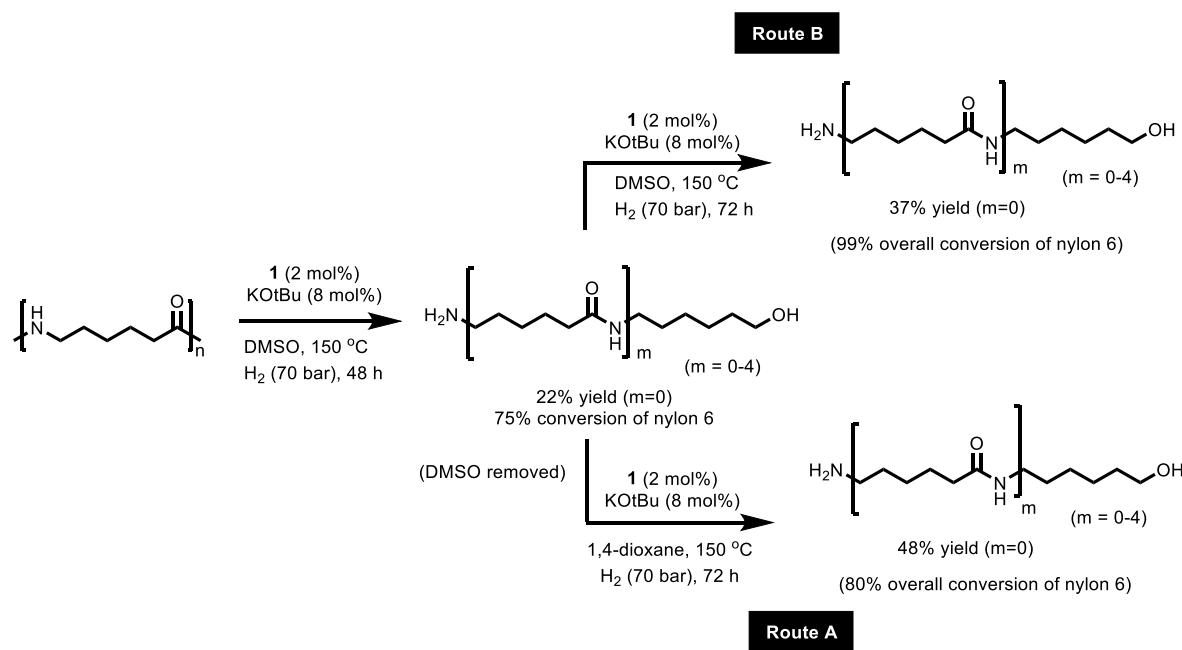
$$\sqrt[3]{\frac{M_2}{M_1}} < \frac{D_1}{D_2} < \sqrt[2]{\frac{M_2}{M_1}}$$

For linear molecules:

$$\frac{D1}{D2} \approx \sqrt[2]{\frac{M2}{M1}}$$

M2/M1 = 2.8

9. Sequential hydrogenation of nylon 6



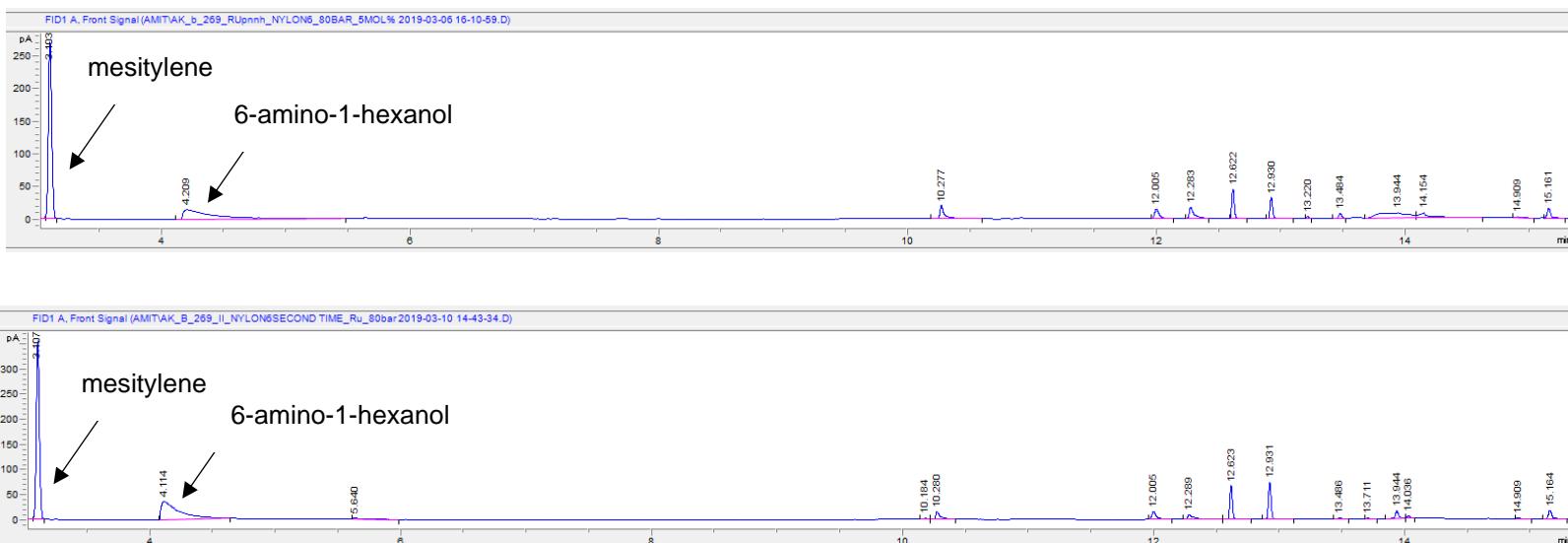


Fig. S12. GC taken after first hydrogenation (top) and second hydrogenation (bottom) steps (route B).

Route A: Complex **1** (10 mg, ~0.02 mmol) and KOtBu (9 mg, 0.08 mmol) were dissolved in the given solvent (2.5 mL) to which resins of nylon 6 (~117 mg, 1 mmol relative to the monomer) was added. The reaction mixture was transferred to an autoclave and pressurized with H₂ (70 bars). The autoclave was heated at 150 °C under continuous stirring for 48 h. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood. Mesitylene (120 mg, 1 mmol) was added to the reaction mixture as an internal standard and the reaction mixture was analysed by GC, ESI-MS and ¹H NMR spectroscopy. The yield of 6-amino-1-hexanol was determined by GC using mesitylene as an internal standard. DMSO was removed and the conversion of nylon 6 was determined by the weight measurement as per the procedure described above (section 2). 1,4-dioxane (3 mL) was added to the mixture of complex **1** (10 mg, ~0.02 mmol) and KOtBu (9 mg, 0.08 mmol). The resulting dioxane solution was added to the residue obtained after removal of the DMSO. The resulting suspension was transferred to an autoclave and pressurized with H₂ (70 bars). The autoclave was heated at 150 °C under continuous stirring

for 72 h. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood. Mesitylene (120 mg, 1 mmol) was added to the reaction mixture as an internal standard and the reaction mixture was analysed by GC, ESI-MS and ¹H NMR spectroscopy. The yield of the 6-amino-1-hexanol was determined by GC using mesitylene as an internal standard. Conversion of nylon 6 was determined by the weight measurement as per the procedure described above (section 2).

Route B: Complex **1** (10 mg, ~0.02 mmol) and KOtBu (9 mg, 0.08 mmol) were dissolved in DMSO (2.5 mL) to which resins of nylon 6 (~117 mg, 1 mmol relative to the monomer) was added. The reaction mixture was transferred to an autoclave and pressurized with H₂ (70 bars). The autoclave was heated at 150 °C under continuous stirring for 48 h. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood. Mesitylene (120 mg, 1 mmol) was added to the reaction mixture as an internal standard and the reaction mixture was analysed by GC, ESI-MS and ¹H NMR spectroscopy. Yield of the 6-amino-1-hexanol was determined by the GC using mesitylene as an internal standard. To the same reaction mixture complex **1** (10 mg, ~0.02 mmol) and KOtBu (9 mg, 0.08 mmol) were added. The resulting suspension was transferred to an autoclave and pressurized with H₂ (70 bars). The autoclave was heated at 150 °C under continuous stirring for 72 h. After the reaction time was completed, the autoclave was cooled to room temperature and the hydrogen gas was slowly vented off in a fume hood and the reaction mixture was analysed by GC, ESI-MS and ¹H NMR spectroscopy. Yield of the 6-amino-1-hexanol was determined by the GC using mesitylene as an internal standard. Conversion of nylon 6 was determined by the weight measurement as per the procedure described above (section 2).

10. Isolation of 6-amino-1-hexanol after the hydrogenation of nylon-6 in DMSO

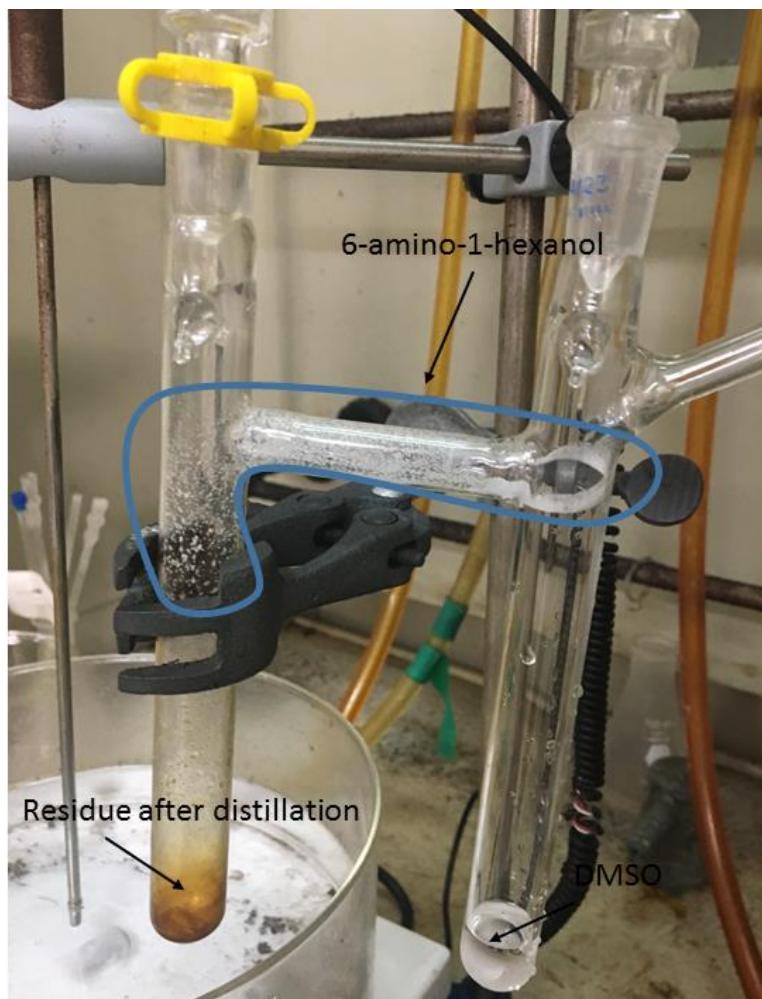


Fig. S13. Setup for the vacuum distillation to separate DMSO and 6-amino-1-hexanol.

After the double hydrogenation step as described in route B of Section 9, the DMSO was removed by vacuum distillation using an H-shaped flask as described in Fig. S13. DMSO was first removed at 80 °C (vacuum: in the range of 10⁻² bar) after which the temperature was raised to 100 °C. At this temperature under dynamic vacuum (in the range of 10⁻² bar) 6-amino-1-hexanol was deposited as white crystals on the walls of the H-shaped flask as shown in Fig. S13. DMSO was removed first by pipette from the right tube and then the crystals of 6-amino-1-hexanol were separated by a thin-long spatula. Isolated yield: 37 mg, 31%. The ¹H

NMR and ESI-Mass spectra of the isolated 6-amino-1-hexanol were recorded which are in agreement with the reported spectra.⁹

¹H NMR (400.36 MHz, CDCl₃, 298 K): δ 3.67 (t, ³J_{HH} = 6.6 Hz, 2H, CH₂O), 2.72 (t, ³J_{HH} = 7.6 Hz, 2H, CH₂N), 1.60-1.40 (m, 8H, CH₂), 1.27 (br, 2H, NH₂).

MS (ESI/TOF): *m/z* calcd for C₆H₁₆NO [M+H]⁺: 117.11; found: 117.11.

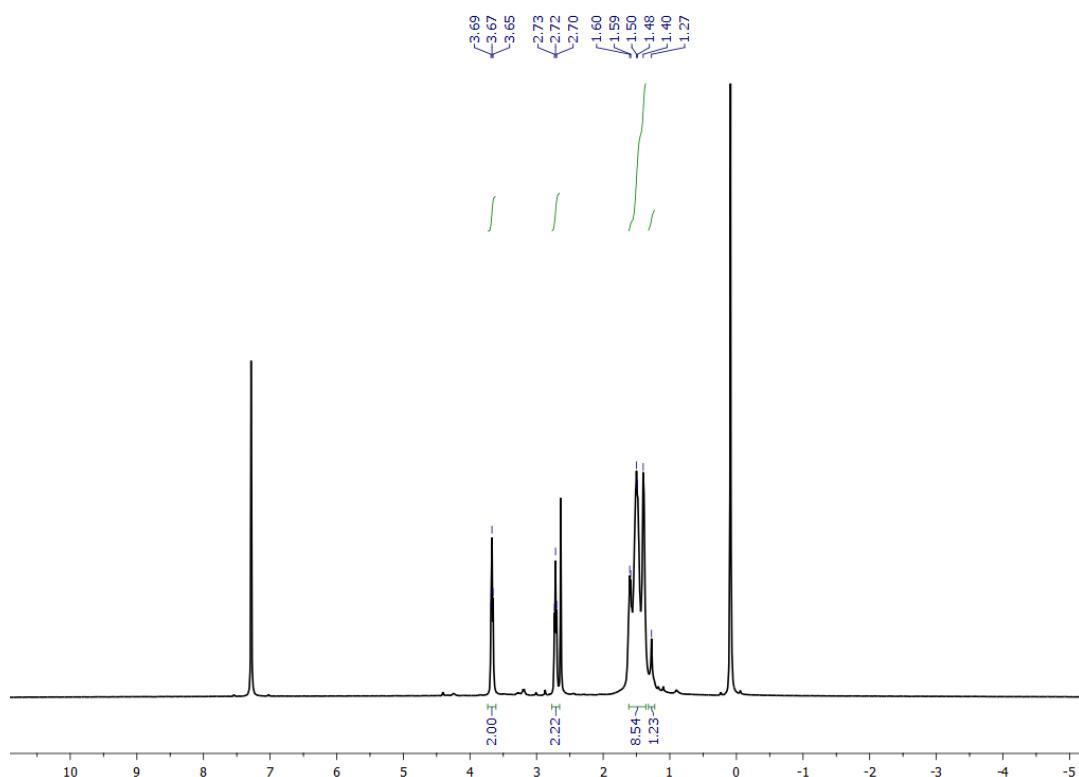


Fig. S14 A. ¹H NMR (400.36 MHz, CDCl₃, 298 K) spectrum of the isolated 6-amino-1-hexanol; signals at δ 2.6 and 0.09 are due to residual DMSO and grease signals, respectively.

Scale-up experiment: A scale-up (4 times) experiment was performed using the above described method. Complex **1** (40 mg, ~0.08 mmol) and KO^tBu (36 mg, 0.32 mmol) were dissolved in DMSO (10 mL) to which resins of nylon 6 (~468 mg) was added. The reaction mixture was transferred to an autoclave and pressurized with H₂ (70 bars). The autoclave was heated at 150 °C under continuous stirring for 48 h. After the reaction time was completed, the autoclave was cooled to room

temperature and the hydrogen gas was slowly vented off in a fume hood. The autoclave was then taken to the glove box and to the same reaction mixture complex **1** (40 mg, ~0.08 mmol) and KO^tBu (36 mg, 0.32 mmol) were added. The autoclave was pressurized with H₂ (70 bars) and heated at 150 °C under continuous stirring for 72 h. Removal of DMSO and isolation of 6-amino-1-hexanol was performed according to the method described above (Fig S13) which resulted in ~160 mg (34% yield) of 6-amino-1-hexanol.

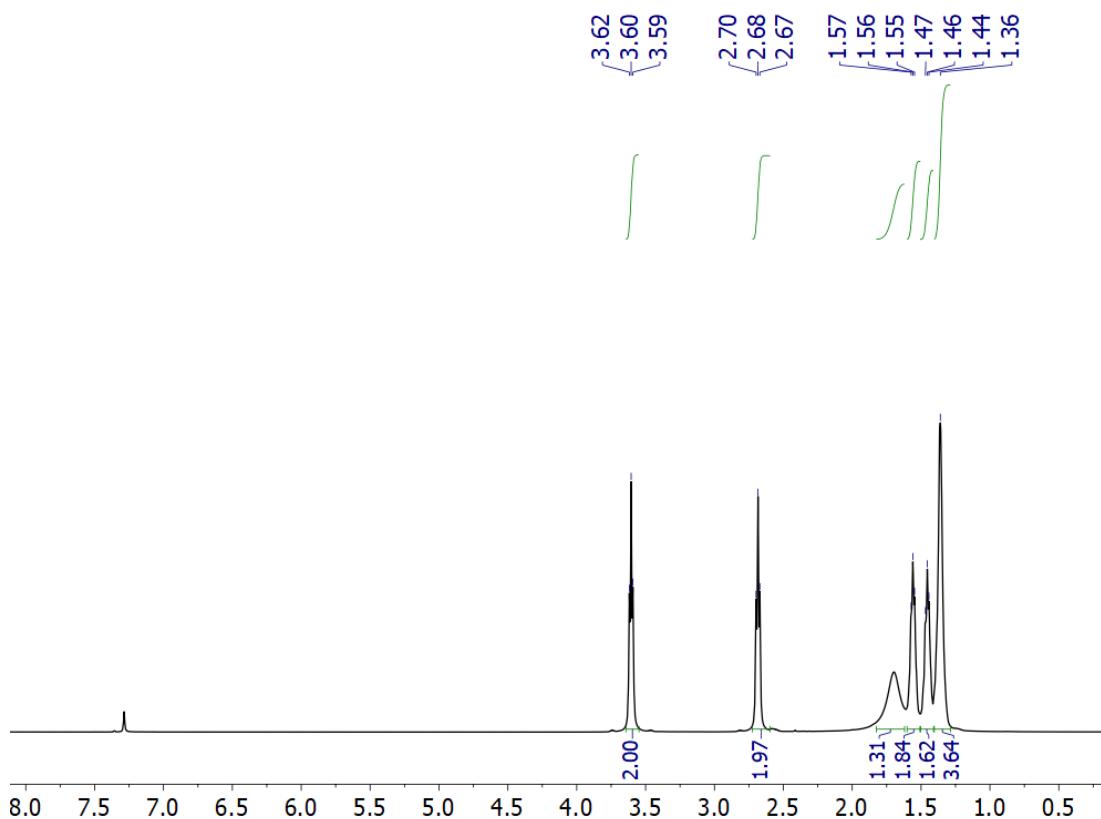


Fig. S14 B. ¹H NMR (400.36 MHz, CDCl₃, 298 K) spectrum of the isolated 6-amino-1-hexanol on scale-up.

Preliminary energy calculation for the removal of DMSO: As our procedure for the product isolation or sequential hydrogenation strategy (route A, section 9) involves removal of DMSO, we did a preliminary calculation to know how much energy is required for the removal of DMSO. Energy needed for the removal of DMSO can be calculated by adding the energy needed by DMSO to reach boiling and enthalpy of vaporization.

$$\begin{aligned}
 Q \text{ (energy/mol)} &= Cp\Delta T + \Delta Hv \\
 &= 149.39 \text{ (Jmol}^{-1}\text{K}^{-1}\text{)}^* (65 \text{ K}) + 48.1 \text{ (kJmol}^{-1}\text{)} \\
 &= 57.81 \text{ kJmol}^{-1}
 \end{aligned}$$

$\Delta T = 363 \text{ K}$ (Avg of 80-100 °C, the temperature for removal of DMSO) – 298 K

Values of C_p and ΔH_v have been taken from the NIST database (<https://webbook.nist.gov/cgi/cbook.cgi?ID=C67685&Mask=2>) and *J. Chem. Technol. Biotechnol.*, **1987**, 37, 145-152.

No of moles in 2.5 mL of DMSO = 0.035 mol

Energy required for the removal of 2.5 mL DMSO = 2.02 kJ

11. Measurement of the molecular weight of the nylons (polyamides)

The molecular weight of nylon 6 resins (size 3 mm, purchased from Sigma-Aldrich) was found by a personal communication with the technical team of Sigma-Aldrich. The molecular weight of Nylon 6 powder (purchased from the Goodfellow) was determined by measuring the intrinsic viscosity of the polymer using Ostwald's viscometer and by applying Mark-Houwink-Sakurada equation: $[\eta] = K (M_v)^\alpha$, where η is the intrinsic viscosity and M_v is the viscosity average molecular weight.¹⁰ K and α are the are two parameters that depend on the solvent, polymer, and temperature.

Measurement of Intrinsic viscosity: Nylon 6 (20 mg) was dissolved in meta-cresol (27 mL) by stirring at room temperature for 6-8 hours to obtain a concentration of ~0.075 g/dL. The nylon solution was added to Ostwald's viscometer and time of flow (t_{nylon}) between the marked lines was measured with a stop watch. Similarly, the time of flow for the solvent ($t_{solvent}$) meta cresol was measured. Two additional nylon solution of concentrations 0.05 and 0.025 g/dL were prepared and their time of flow (t_{nylon}) was determined using Ostwald's viscometer.

At low concentration, relative viscosity (η_r) can be calculated as: $\eta_r = t_{nylon}/t_{solvent}$. After calculating relative viscosity (η_r), two additional parameters specific viscosity (η_{sp}) and reduced viscosity (η_{red}) were calculated using following equations:

$\eta_{sp} = \eta_r - 1$ and $\eta_{red} = \eta_{sp}/C$ (C = concentration). Intrinsic viscosity is defined as the reduced viscosity at zero concentration. Therefore, the specific viscosity was plotted against concentration and the intercept was measured to be the intrinsic viscosity.

Time of flow for the solvent meta cresol (t_{solv}) = 1294 sec

Table S7. Parameters for measuring the viscosity avg molecular weight of nylon 6.

Conc (g/dL)	t_{nylon}	$\eta_{sp} = \eta_r - 1$	$\eta_{red} = \eta_{sp}/C$
0.1	1876	0.45	4.5
0.075	1633	0.262	3.5
0.05	1475	0.14	2.8

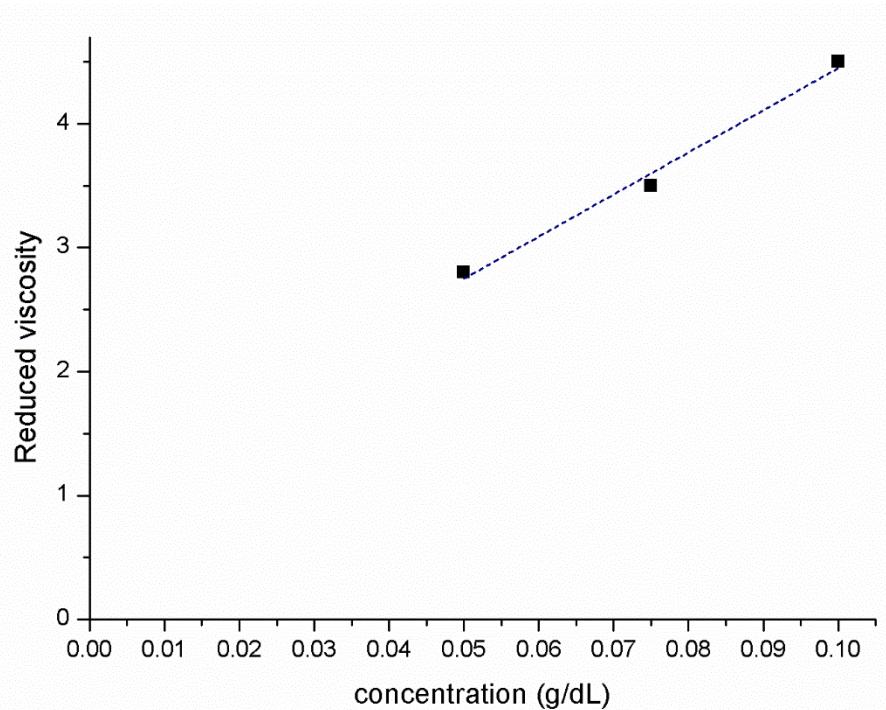


Fig. S15. Plot of reduced viscosity relative to the concentration of nylon 6. Intercept: 4.1.

Intrinsic viscosity from the graph $[\eta] = 1.05$

From, Mark-Houwink-Sakurada equation: $[\eta] = K (M_v)^\alpha$

For nylon 6 in meta cresol at 25 °C, values of $K = 3.2 \times 10^{-3}$ dl/g and $\alpha = 0.62^{10}$

$$\log(1.05) = -3 + \log(3.2) + 0.62 \log(M_v)$$

$$M_v = \sim 11000$$

12. Spectral details of the catalytic hydrogenation of other polyamides

12.1 NMR spectra of the isolated polyamides

The synthesis and the determination of molecular weight of the remaining polyamides (Entries 4-8, Table 2 of the manuscript) were performed according to the method reported by us earlier.¹ NMR spectra of these polyamides are presented here:

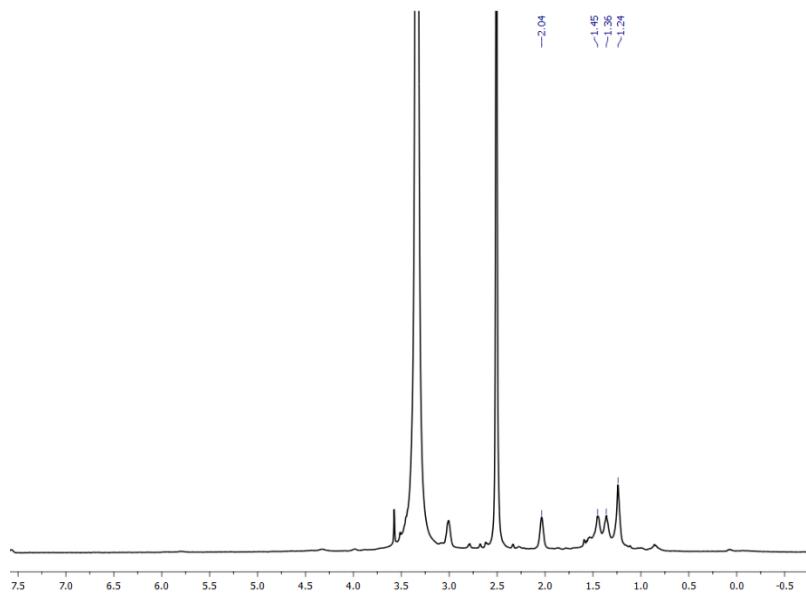


Fig. S16. ¹H NMR (500.08 MHz, 298 K, DMSO-d₆) spectrum of the synthesized polyamide (Table 2, entry 4).

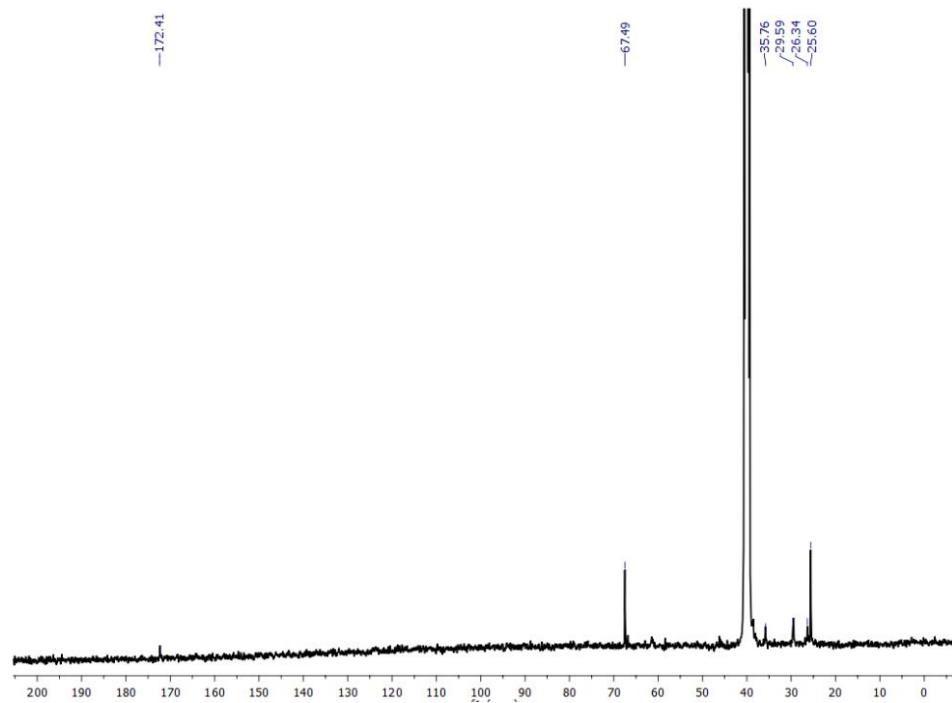


Fig. S17. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298 K, DMSO-d₆) spectrum of the synthesized polyamide (Table 2, entry 4).

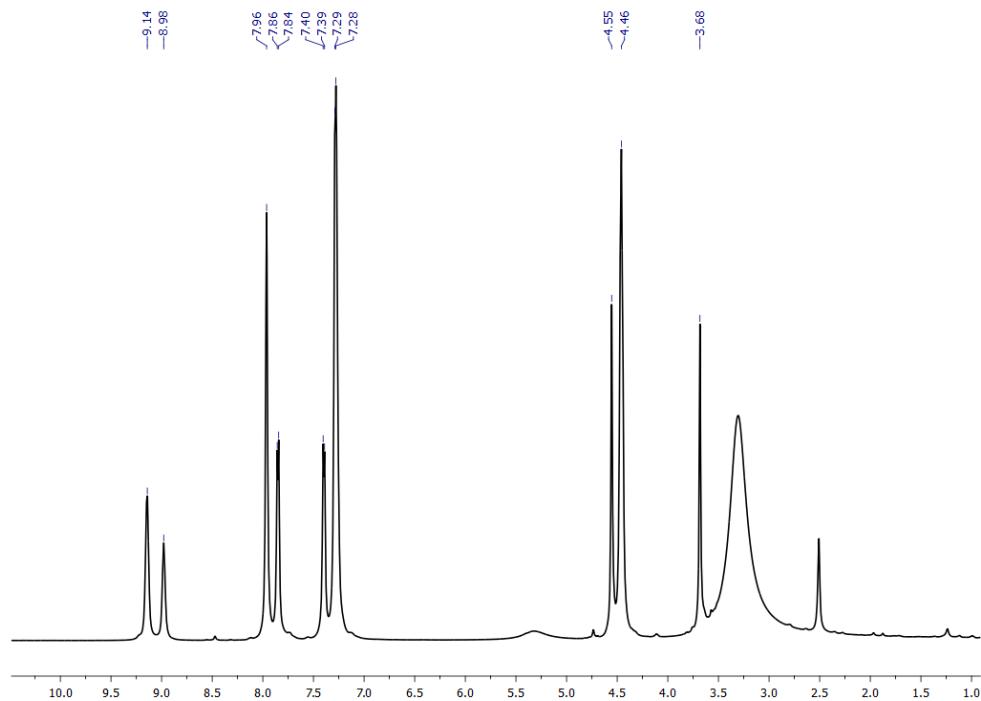


Fig. S18. ^1H NMR (500.08 MHz, 298 K, DMSO-d₆) spectrum of the synthesized polyamide (Table 2, entry 5).

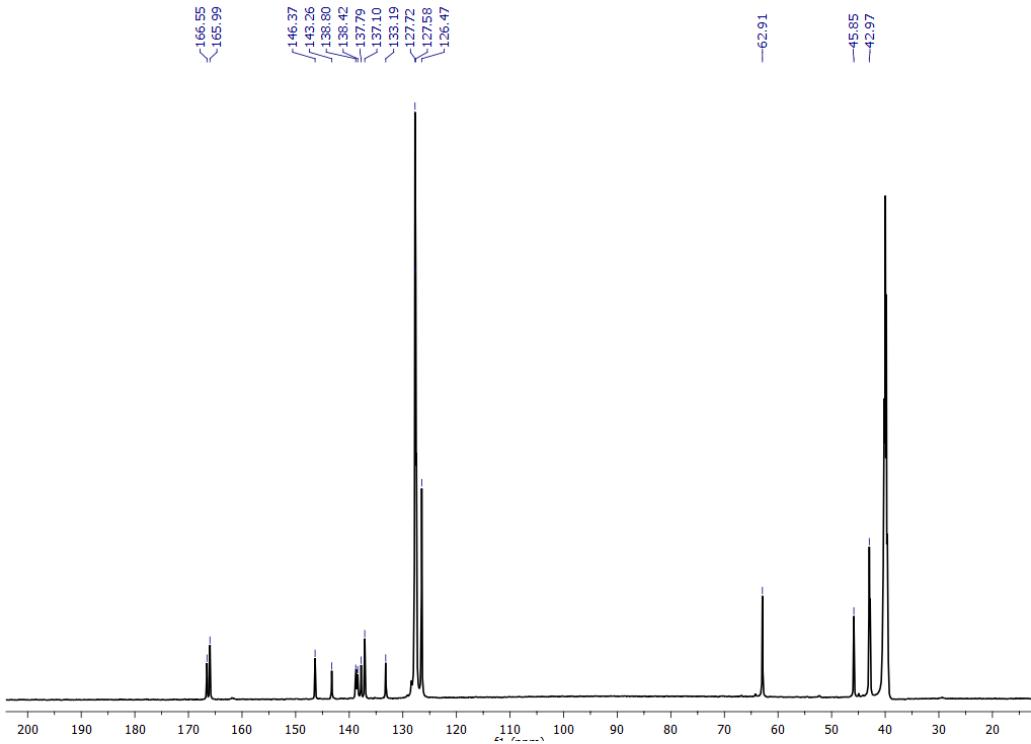


Fig. S19. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298 K, DMSO-d6) spectrum of the synthesized polyamide (Table 2, entry 5).

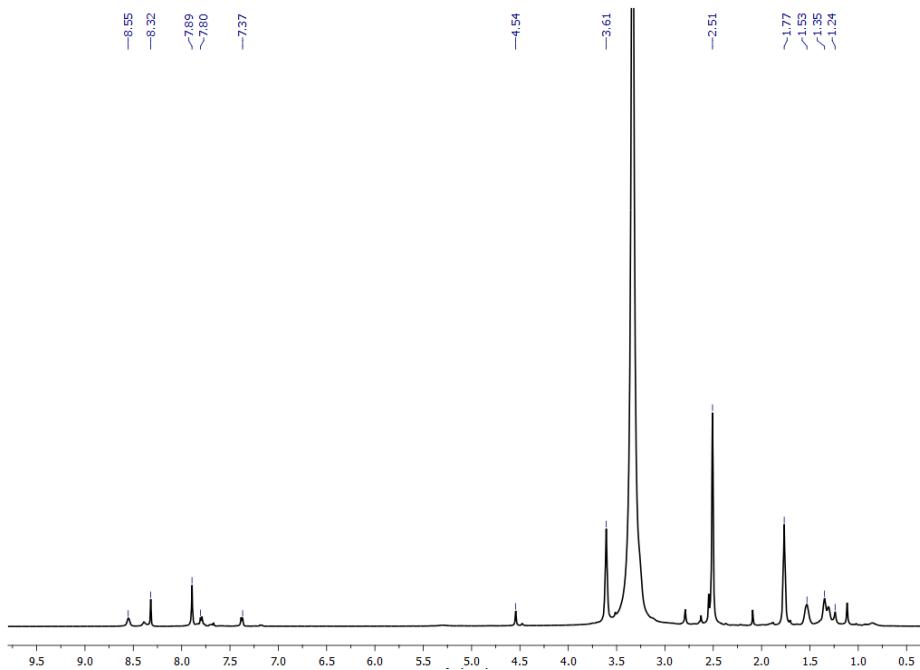


Fig. S20. ^1H NMR (500.08 MHz, 298 K, DMSO-d6) spectrum of the synthesized polyamide (Table 2, entry 6).

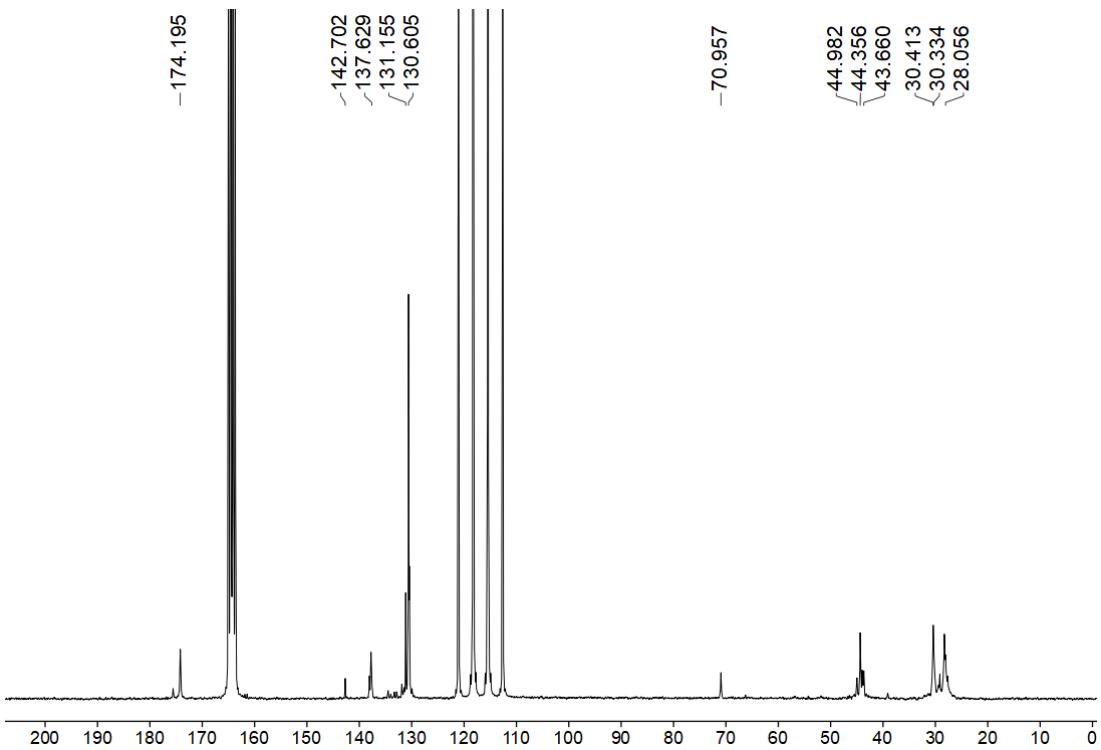


Fig. S21. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298 K, CF_3COOD) spectrum of the synthesized polyamide (Table 2, entry 6).

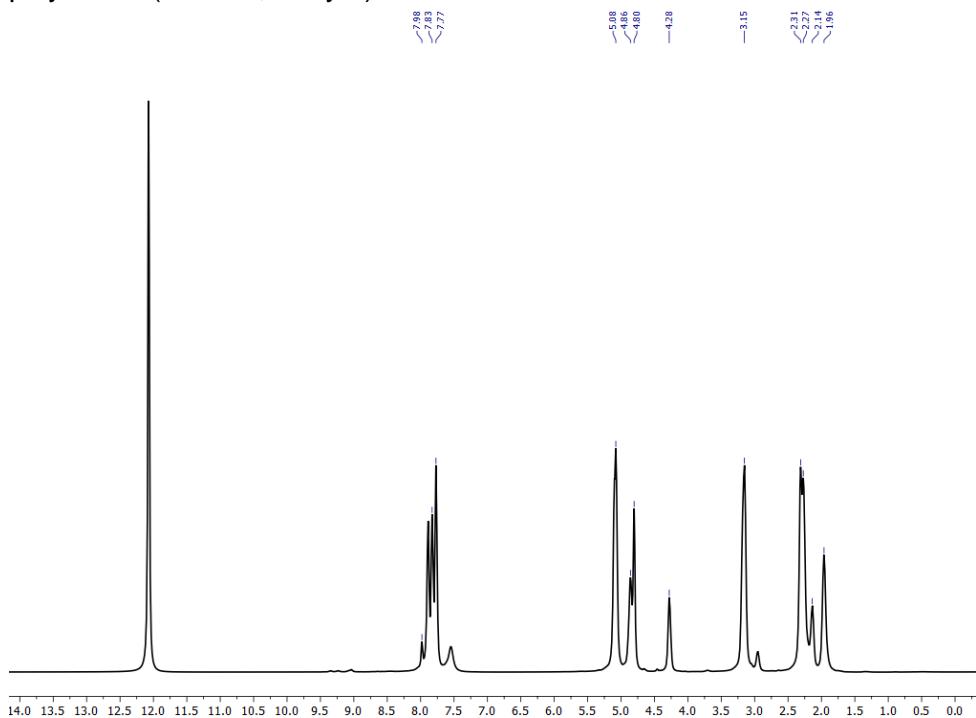


Fig. S22. ^1H NMR (500.08 MHz, 298 K, CF_3COOD) spectrum of the synthesized polyamide (Table 2, entry 7).

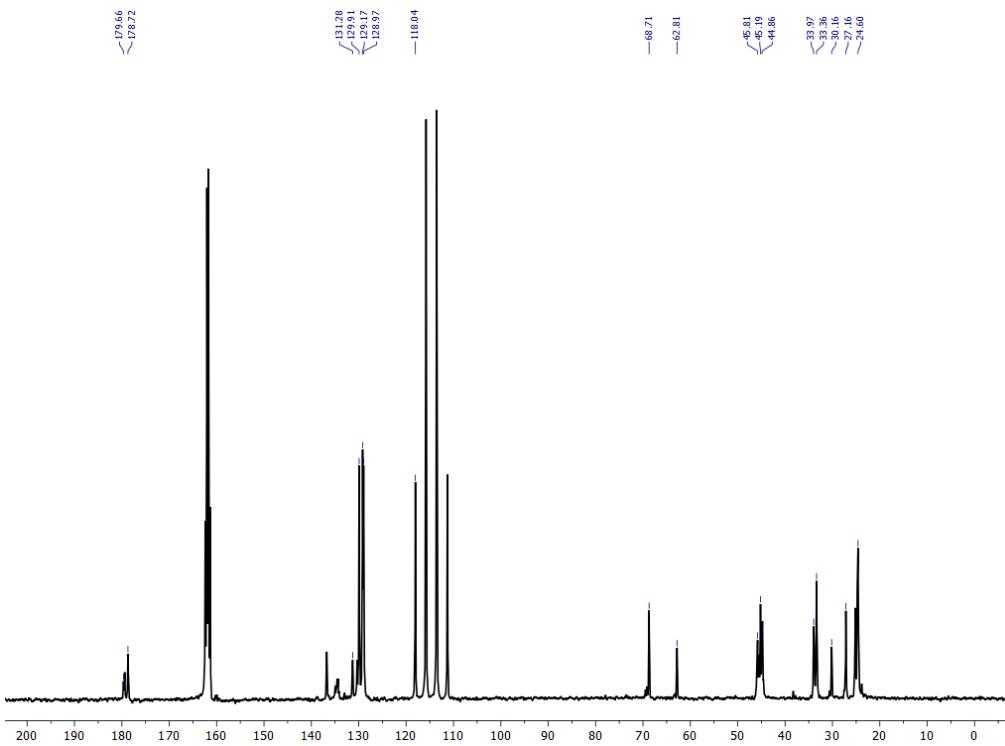


Fig. S23. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298 K, CF_3COOD) spectrum of the synthesized polyamide (Table 2, entry 7).

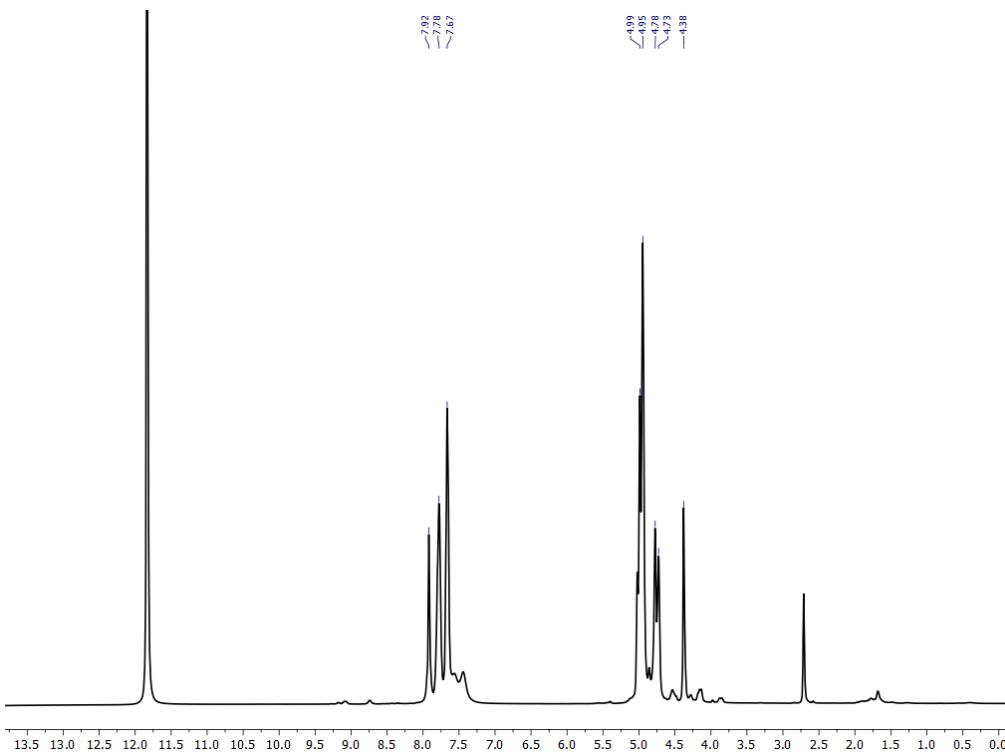


Fig. S24. ^1H NMR (500.08 MHz, 298 K, CF_3COOD) spectrum of the synthesized polyamide (Table 2, entry 8).

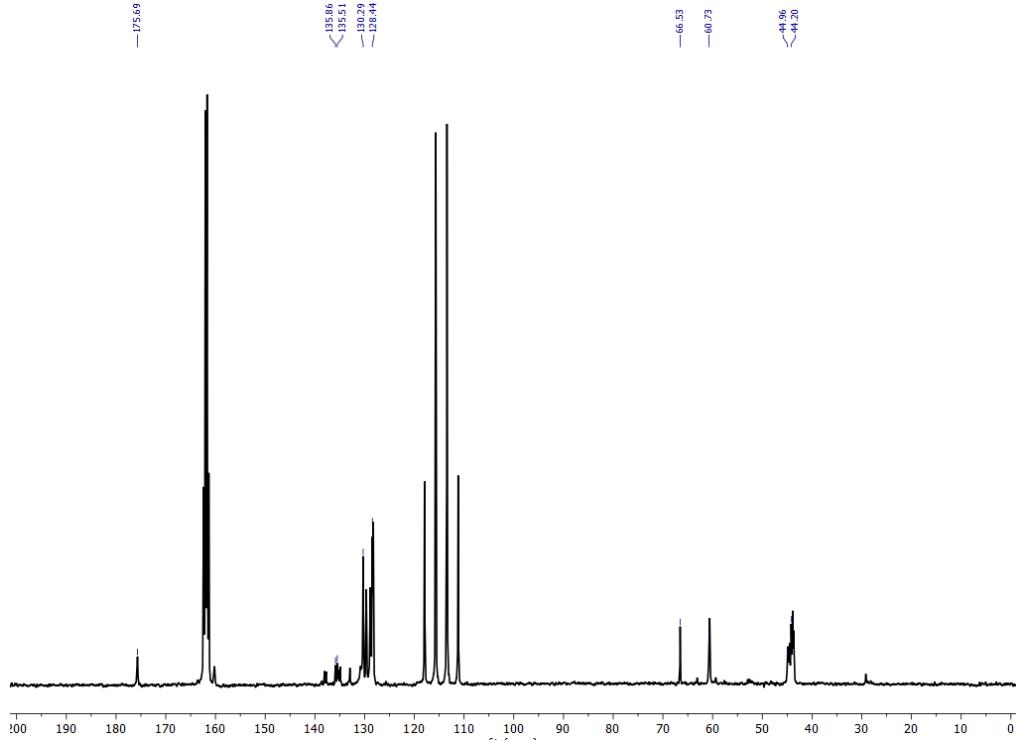
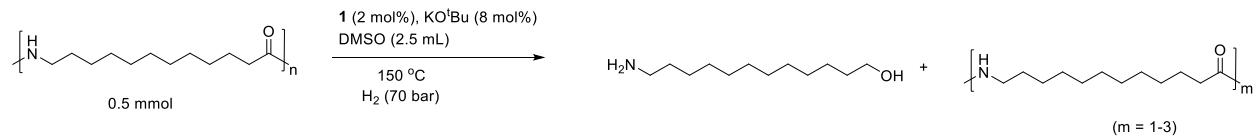


Fig. S25. $^{13}\text{C}\{\text{H}\}$ NMR (125.75 MHz, 298 K, CF_3COOD) spectrum of the synthesized polyamide (Table 2, entry 8).

12.2 GC/ESI-MS details of the catalytic hydrogenation of other polyamides



	complex (mol%)	Base (mol%)	conversion	Amino- alcohol	Oligoamide detection
1	1 (2 mol%)	KOtBu(8 mol%)	80%	30%	yes
2	2 (2 mol%)	KOtBu(8 mol%)	82%	29%	yes

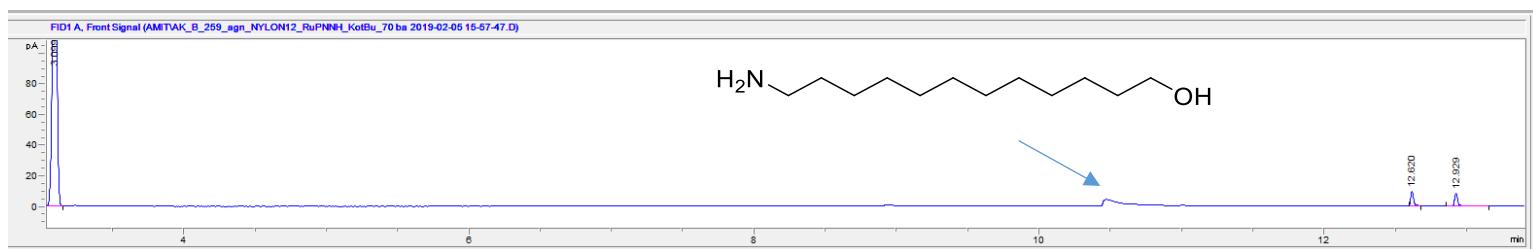


Fig. S26. GC of the reaction mixture after hydrogenation of nylon 12 (Table 2, entry 3).

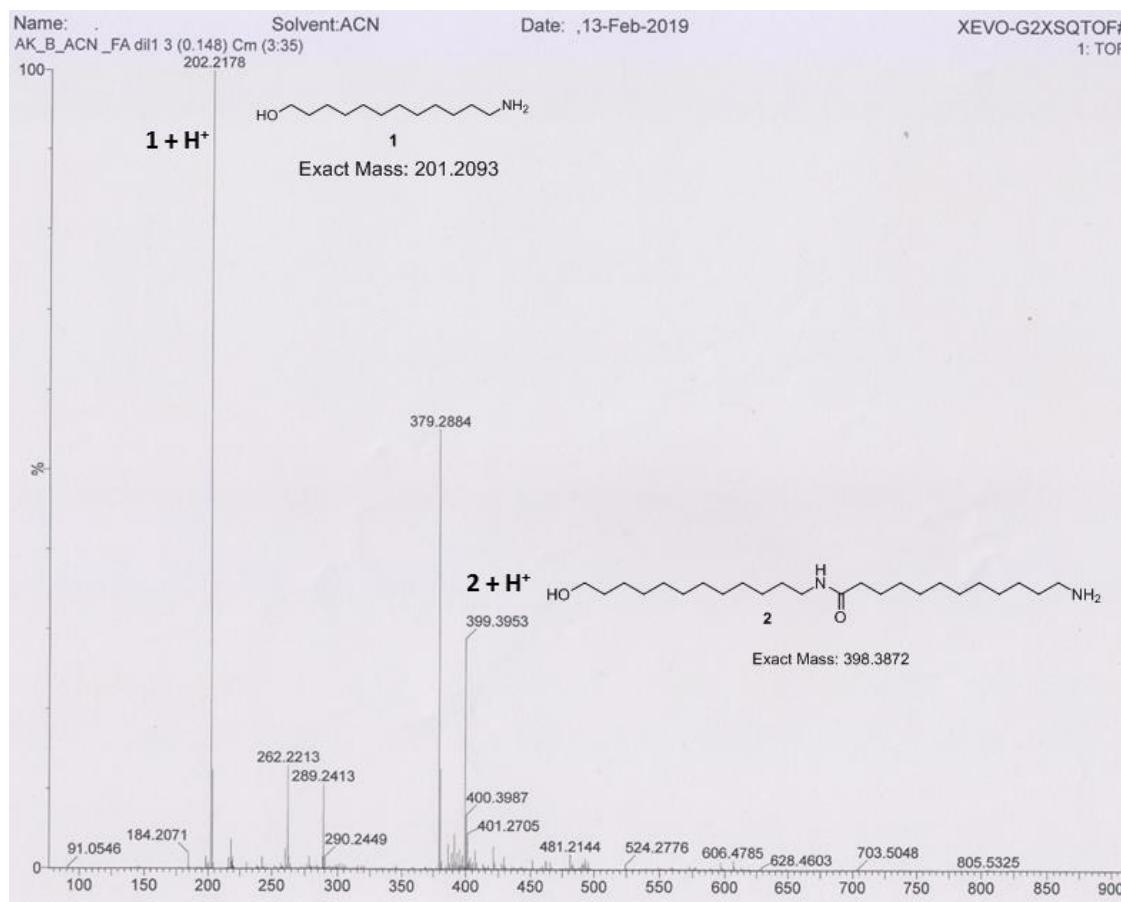


Fig. S27. HR-ESI-MS of the reaction mixture after hydrogenation of nylon 12 (Table 2, entry 3).

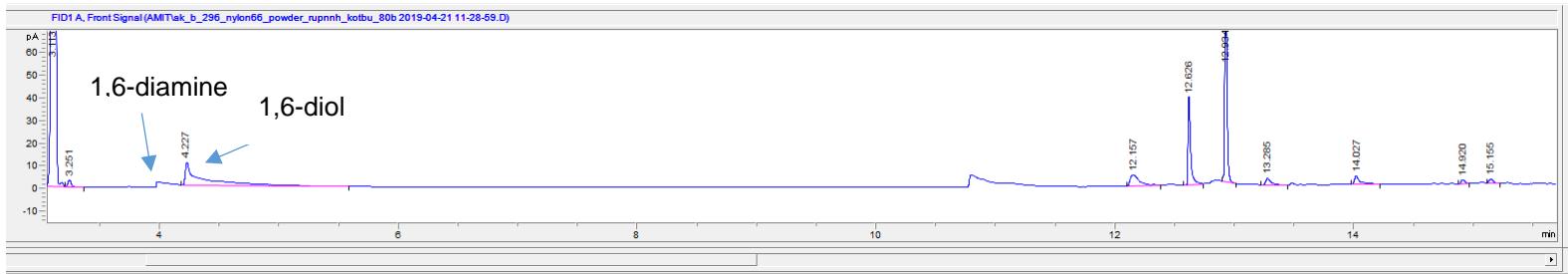
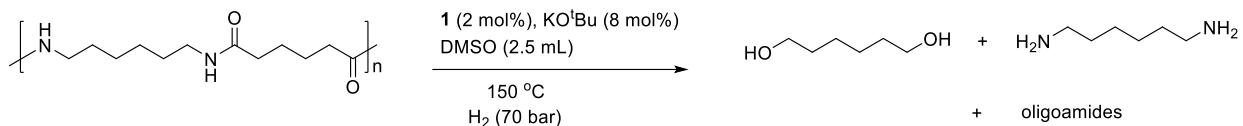


Fig. S28. GC of the reaction mixture after hydrogenation of nylon 66 (Table 2, entry 4)

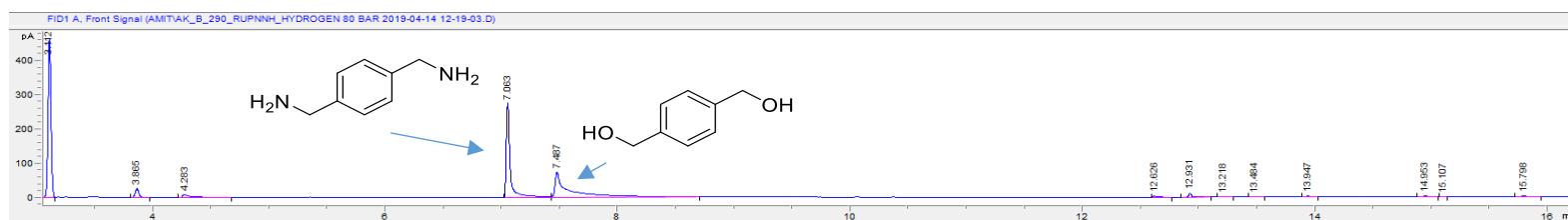
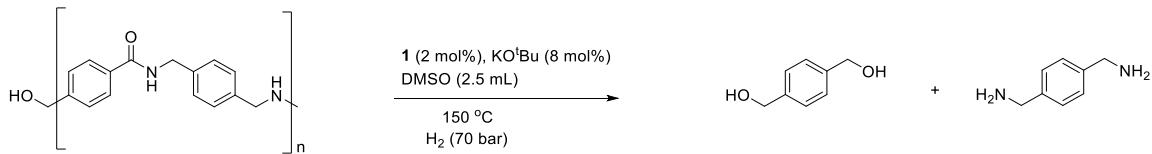


Fig. S29. GC of the reaction mixture after hydrogenation of polyamide (Table 2, entry 5).

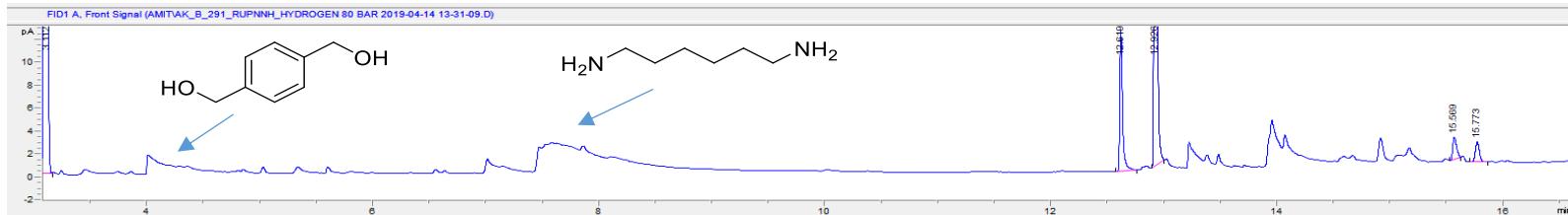
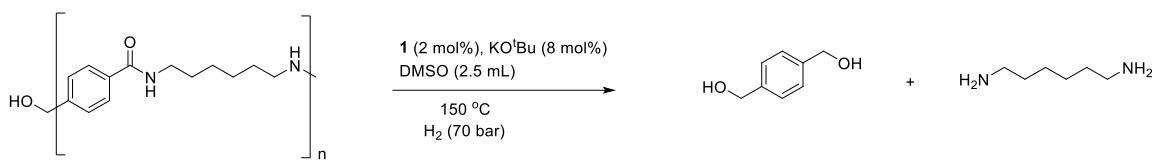


Fig. S30. GC of the reaction mixture after hydrogenation of polyamide (Table 2, entry 6).

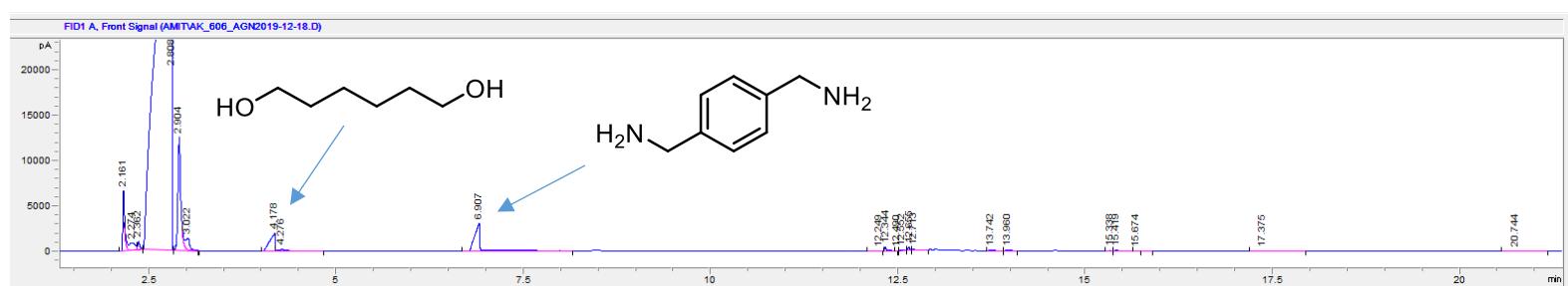
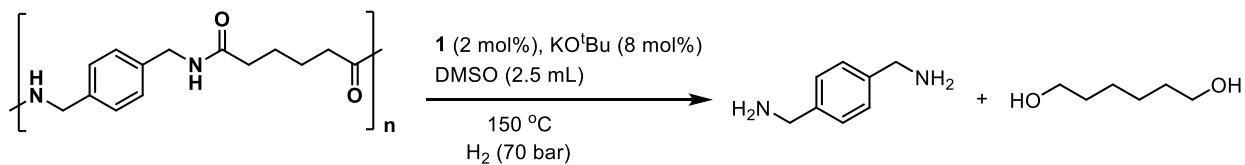


Fig. S31. GC of the reaction mixture after hydrogenation of polyamide (Table 2, entry 7).

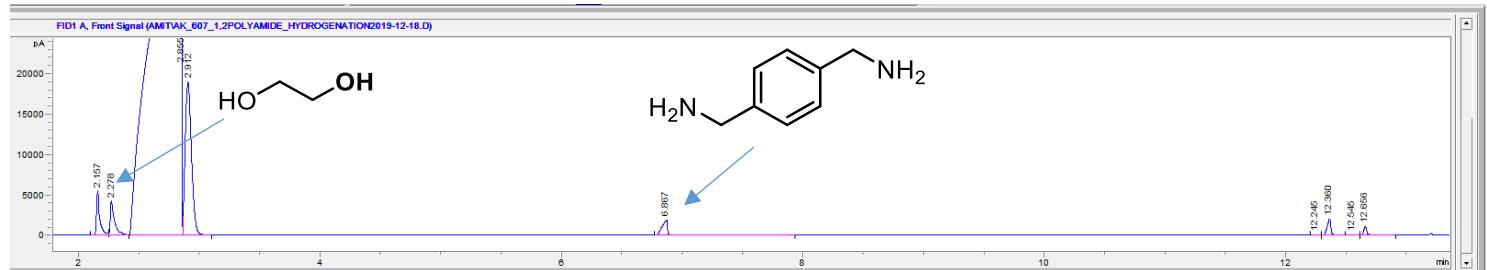
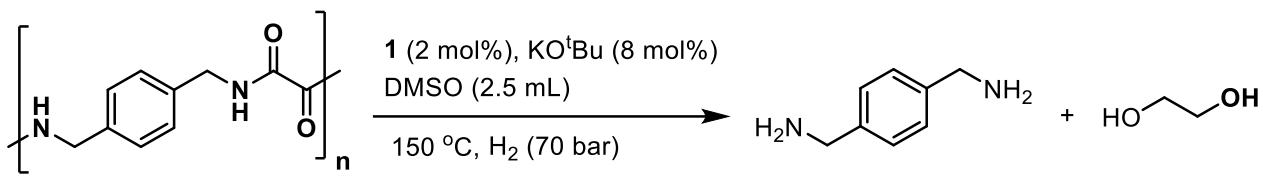


Fig. S32. GC of the reaction mixture after hydrogenation of polyamide (Table 2, entry 8).

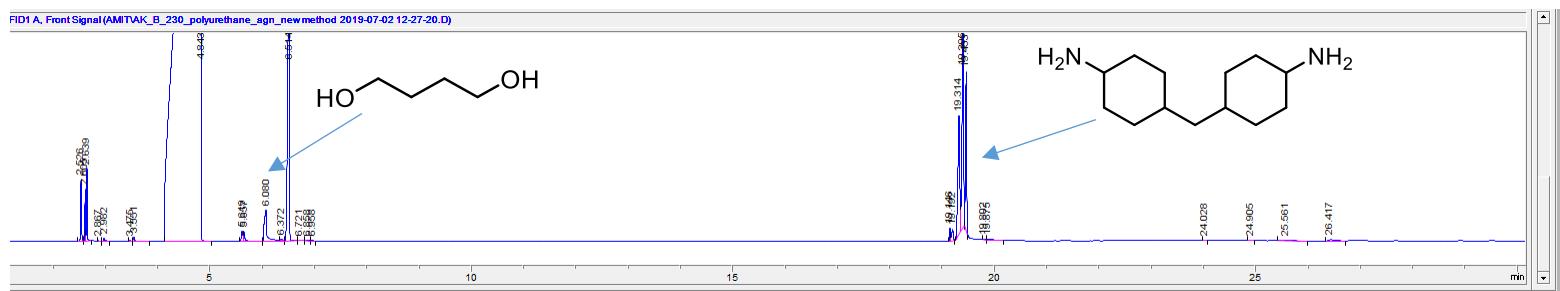
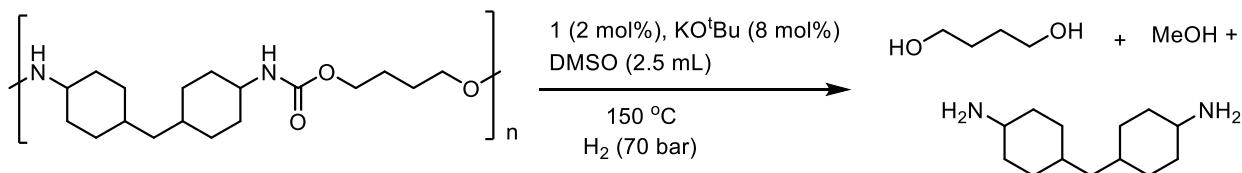
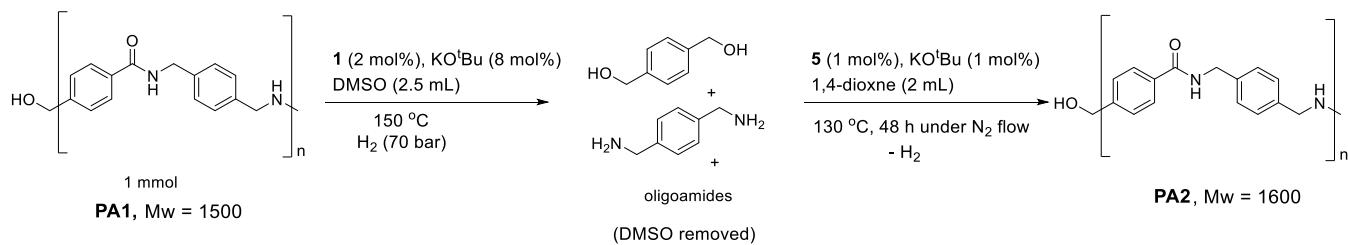
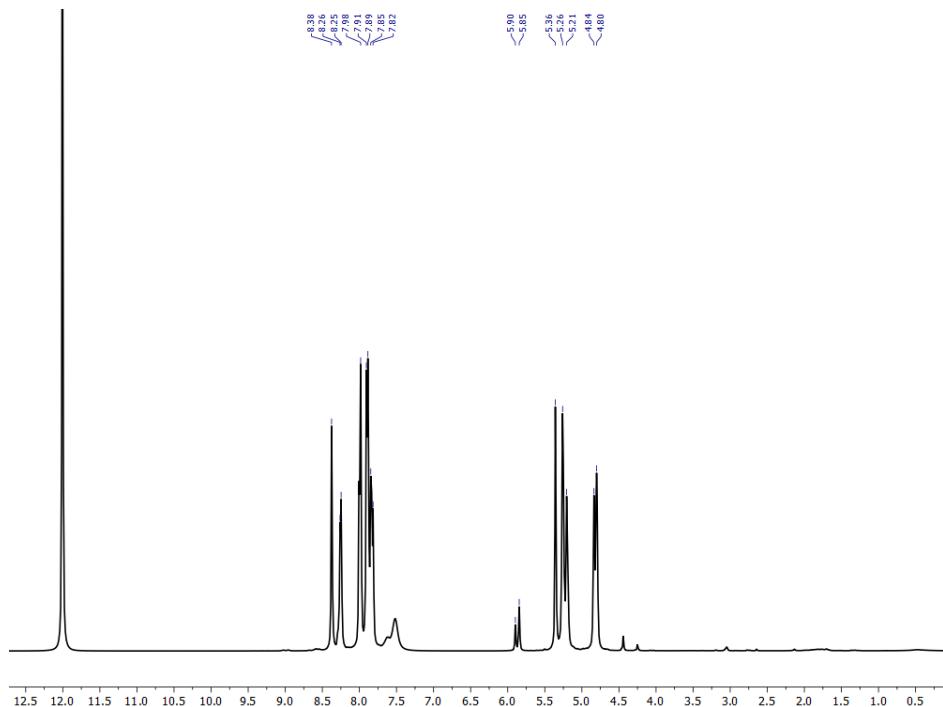


Fig. S33. GC of the reaction mixture after hydrogenation of polyurethane (Table 2, entry 9).

13. Demonstration of the closed loop cycle



As per the conditions described in Table 2, entry 5, an aromatic polyamide (1 mmol, Mw = 1500) was hydrogenated to produce 1,4-benzenedimethanol and p-xylenediamine in 77% and 82% yields, respectively. DMSO was removed by vacuum distillation and the residue was dissolved in 1,4-dioxane (1.5 mL) and transferred to a Schlenk tube. In a separate vial, complex **5** (1 mol%) and KO^tBu (1 mol%) was added to 0.5 mL 1,4-dioxane. The resulting catalytic solution was transferred to the Schlenk tube containing 1,4-dioxane solution of diol and diamine. The Schlenk tube was heated to refluxed under open system with continuous N₂ flow for 48 h forming a white precipitate which was analysed by NMR spectroscopy and ESI-MS.



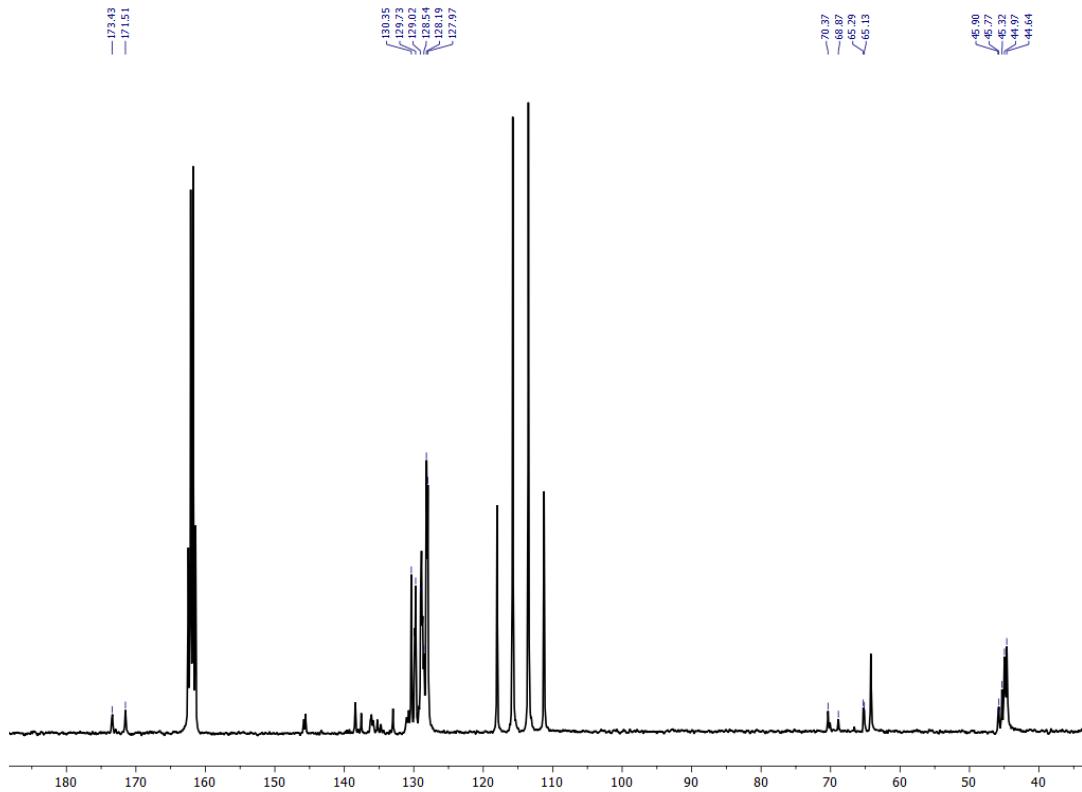


Fig. S35. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.75 MHz, 298 K, CF_3COOD) spectrum of the polyamide **PA 2**.

TOF/TOF™ Reflector Spec #1 MC[BP = 443.3, 12910]

3/3

Sample name: A.R.-189
laser: 550A

Zoom 2

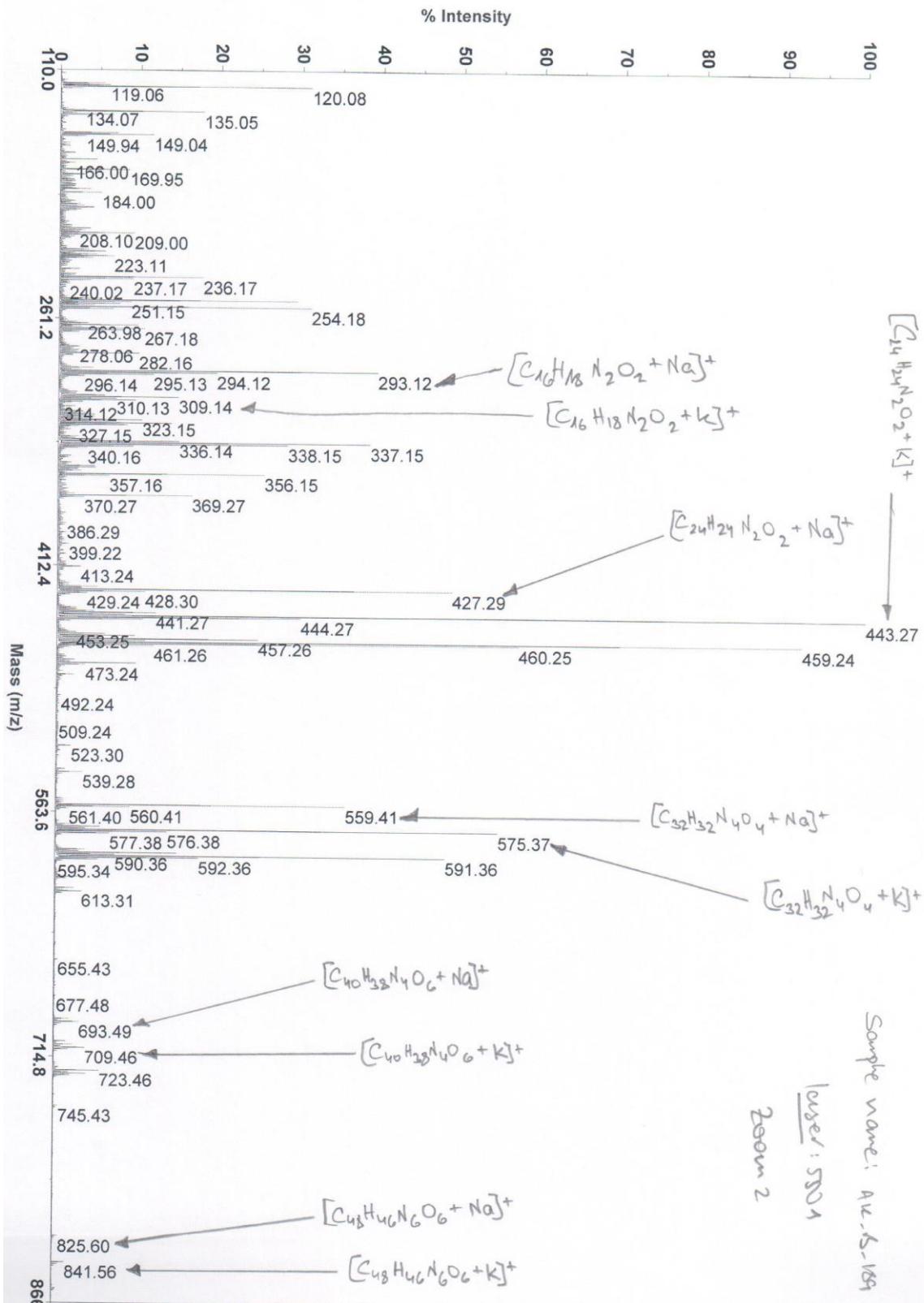
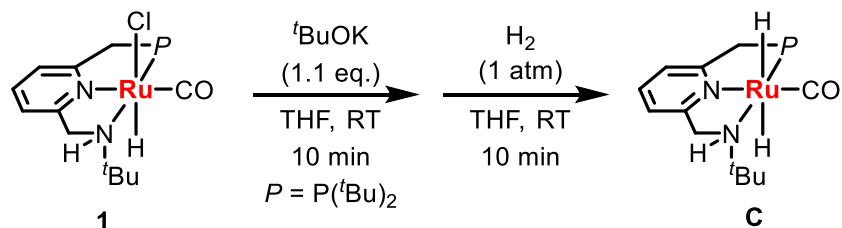


Fig. S36. HR-ESI-MS of the polyamide **PA 2**.

14. Mechanistic Studies

14.1. Synthesis and characterization of complex C



In a glovebox, **1** (19.5 mg, 0.04 mmol) and KO*t*Bu (4.9 mg, 0.044 mmol) were suspended in THF (0.5 mL) in a 5.0 mL vial. After stirring at room temperature for 10 min, the resulting solution was transferred into a J. Young valve NMR tube and treated with 1 atm dihydrogen. The color of the solution immediately changed from dark brown to yellow-brown. A parallel reaction in THF-*d*₈ showed that the dihydride complex **C** was formed, which was fully characterized (only stable under an atmosphere of dihydrogen).

NMR Data of Complex **C**:

¹H NMR (500 MHz, THF-*d*₈, 298 K) δ (ppm) = 7.43 (t, ³J_{HH} = 7.7 Hz, 1H, Py-H), 7.17 (d, ³J_{HH} = 7.8 Hz, 1H, Py-H), 7.04 (d, ³J_{HH} = 7.7 Hz, 1H, Py-H), 5.17 (s, 1H, N-H), 4.29 (dd, ⁴J_{HP} = 14.6, ²J_{HH} = 5.6 Hz, 1H, N-CH₂Py), 4.16 (m, 1H, N-CH₂Py), 3.39 (d, ²J_{HH} = 9.0 Hz, 2H, P-CH₂Py), 1.36 (m, 9H, C(CH₃)₃), 1.31 – 1.28 (m, 18H, C(CH₃)₃), -4.73 (d, ²J_{HP} = 14.9 Hz, 1H, Ru-H), -5.12 (d, ²J_{HP} = 17.6 Hz, 1H, Ru-H).

¹³C{¹H NMR} (125 MHz, THF-*d*₈, 298 K) δ (ppm) = 213.45 (d, ²J_{CP} = 16.8 Hz, Ru-CO), 161.03 (d, ²J_{CP} = 4.8 Hz, Py-C), 160.82 (d, ³J_{CP} = 2.2 Hz, Py-C), 134.83 (s, Py-CH), 119.85 (d, ³J_{CP} = 9.1 Hz, Py-CH), 117.17 (s, Py-CH), 56.69 (s, NCH₂Py),

55.30 (s, NC(CH₃)₃), 38.61 (d, ¹J_{CP} = 18.1 Hz, PC(CH₂Py), 35.78 (d, ¹J_{CP} = 13.6 Hz, PC(CH₃)₃), 30.19 (d, ²J_{CP} = 4.5 Hz, PC(CH₃)₃), 29.82 (d, ²J_{CP} = 4.7 Hz, PC(CH₃)₃), 29.21 (s, NC(CH₃)₃).

³¹P{¹H} NMR (202 MHz, THF-*d*₈, 298 K) δ (ppm) = 123.50 (s).

Performing the same reaction in DMSO-*d*6 also gave signals characteristic of the *trans*-hydride complex **C**, for example hydride signals at δ -5.23 (d, ²J_{H,P} = 15.7 Hz) and -5.42 (d, ²J_{H,P} = 16.0 Hz) in ¹H NMR spectrum and a signal at δ 122.4 in the ³¹P{¹H} NMR spectrum. However, the ³¹P{¹H} NMR spectrum showed formation of some other complexes (δ 108.9 and 100.6) that were unidentified and formation of complex **C** was observed in approximately 76% yield.

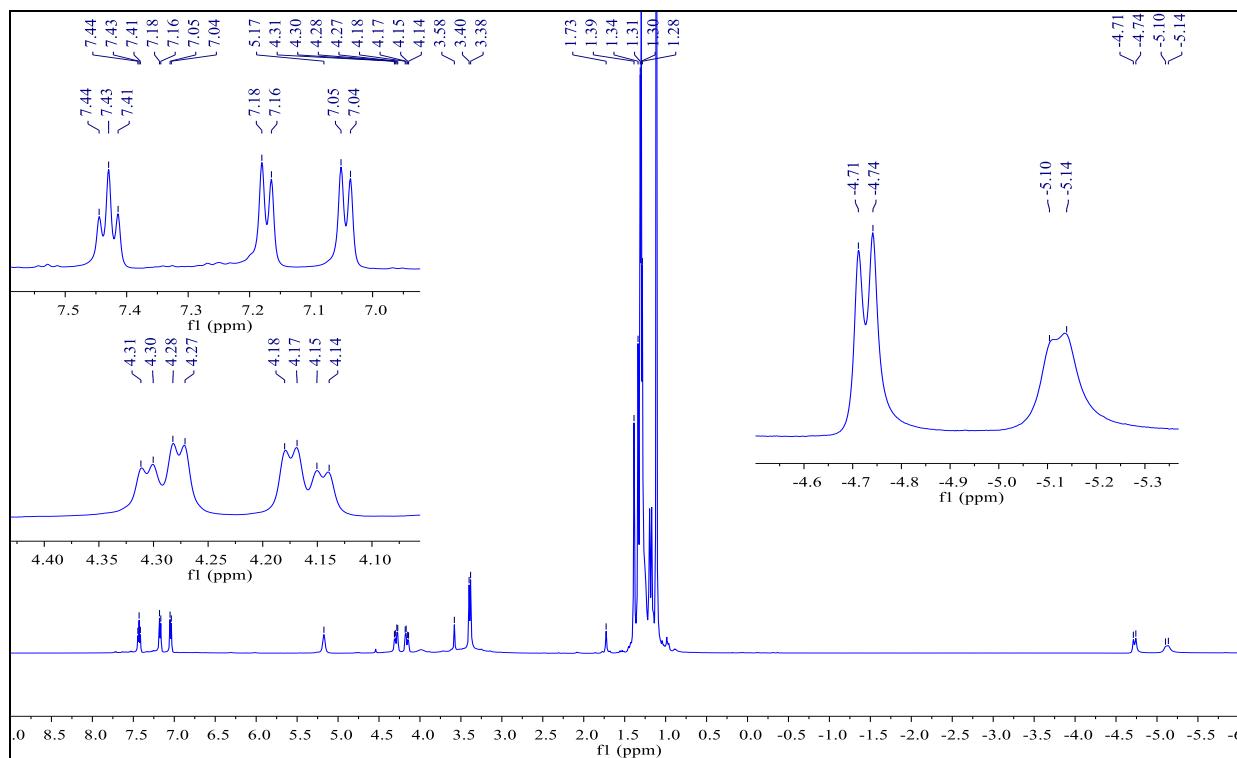


Fig. S37. ¹H NMR (500.08 MHz, THF-*d*₈, 298 K) spectrum of complex **C**.

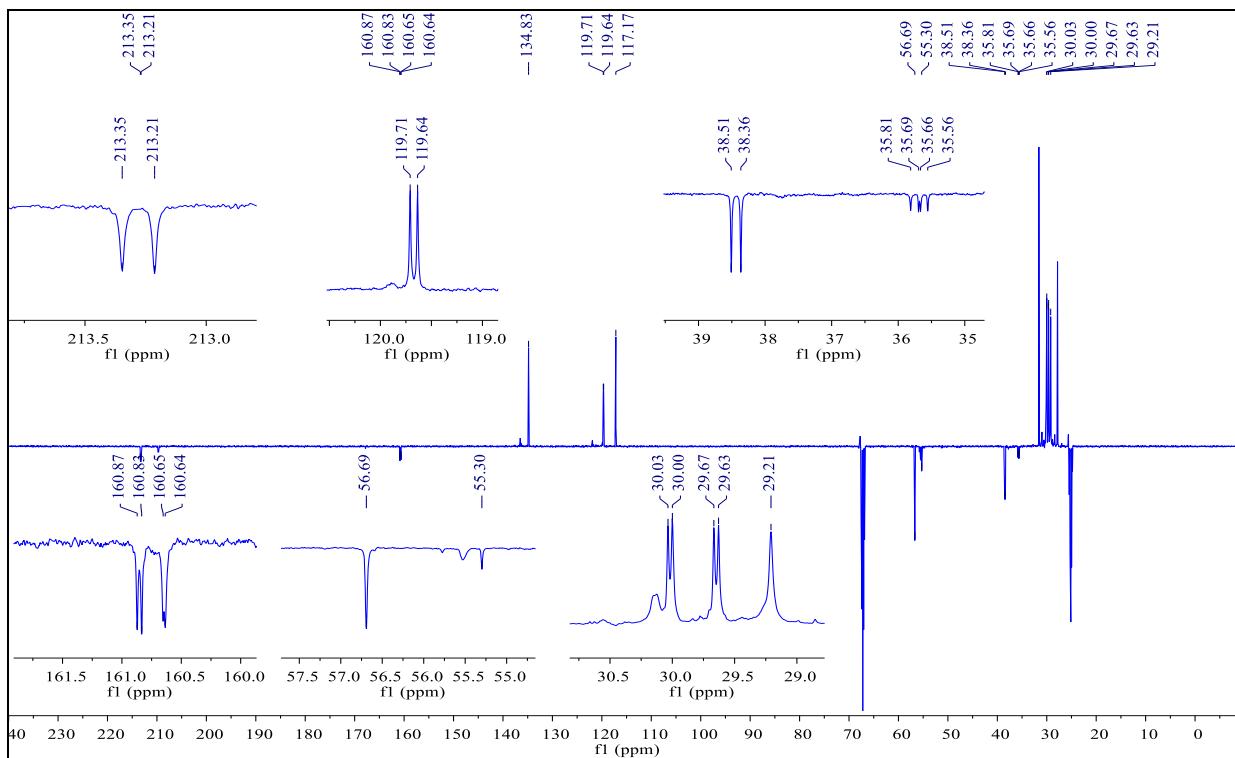


Fig. S38. $^{13}\text{C}\{^1\text{H}\}$ DEPTQ NMR (125.75 MHz, THF- d_8 , 298 K) spectrum of complex **C**.

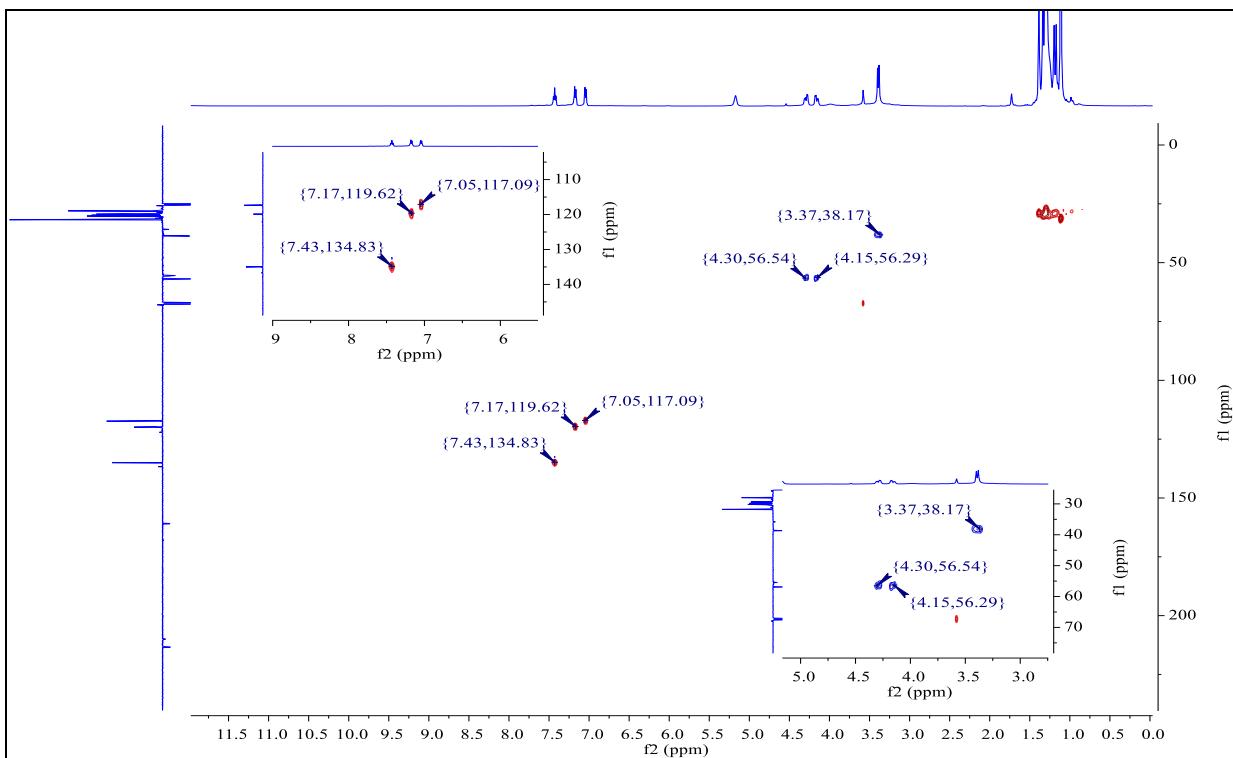


Fig. S39. $^1\text{H}\{^{13}\text{C}\}$ HSQC NMR (500.08 MHz, THF- d_8 , 298 K) spectrum of complex **C**.

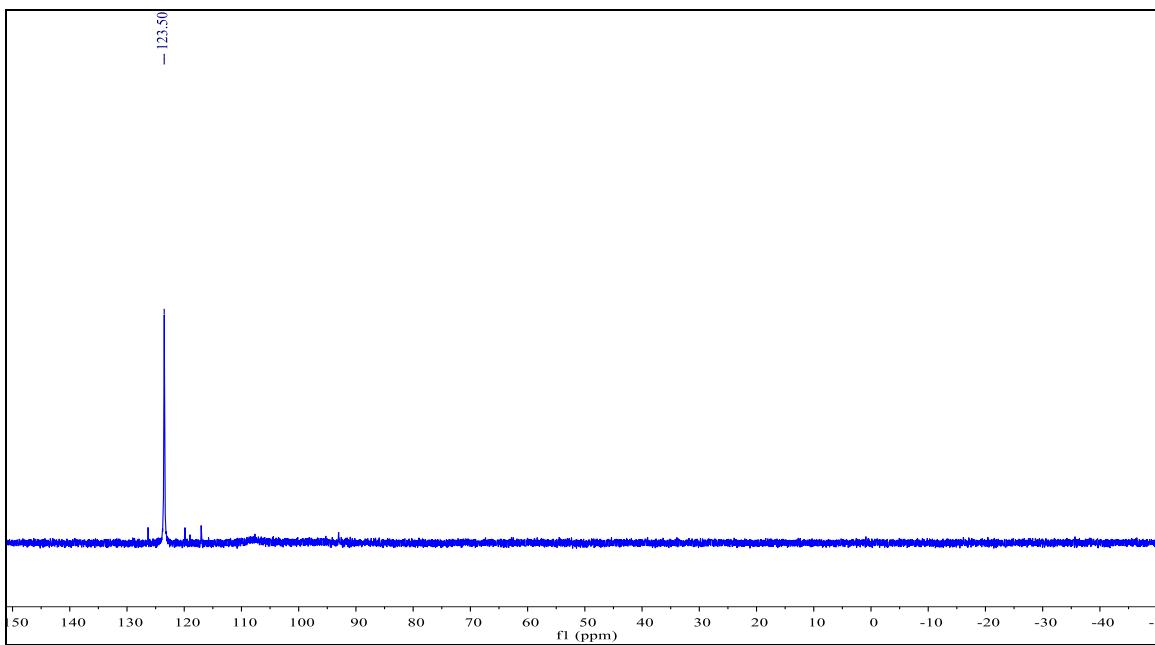
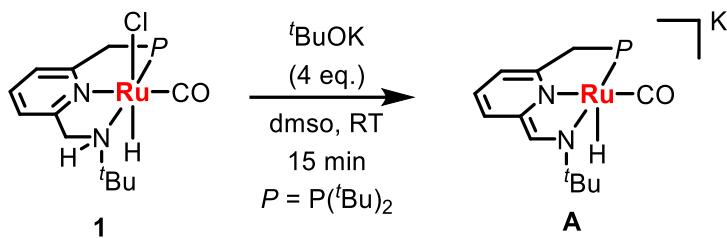


Fig. S40. $^{31}\text{P}\{^1\text{H}\}$ NMR (202.44 MHz, THF- d_8 , 298 K) spectrum of complex **C**.

14.2. Reactivity of complex **1** with KO^tBu in DMSO



Complex **1** reacts with 4 equivalents of base such as KO^tBu in THF to form the doubly deprotonated amido complex **A** characterized and reported earlier by us.² We performed the same reaction in DMSO solvent instead of THF. In a glovebox, **1** (19.5 mg, 0.04 mmol) and KO^tBu (~18 mg, 0.16 mmol) were suspended in DMSO-d6 (0.5 mL). The resulting red solution was transferred to a J. Young valve NMR tube. After 15 minutes the color of the solution turned to dark blue similar to that observed for the synthesis of complex **A** in THF. The ³¹P{¹H} NMR spectrum showed a clean signal at δ 114.0 (d, $J_{\text{H,P}} = 13.0$ Hz) shifted slightly downfield compared to that observed in THF-d8 (δ 124.1, d, $J_{\text{H,P}} = 15.0$ Hz). ¹H NMR spectrum showed a hydride signal at δ -18.19 (d, $J_{\text{H,P}} = 27.0$ Hz, 1H) almost at the same chemical shift as that observed in the case of THF at -18.45 (d, $J_{\text{H,P}} = 28.0$ Hz, 1H). Based on the NMR spectral data we conclude that complex **1** reacts with 4 equivalents of KO^tBu in DMSO to afford the same doubly deprotonated complex **A** as that in case of THF. We also studied the effects of temperature by variable temperature (298 K-400K) NMR experiments on the stability of complex **A** in DMSO-d6. No conclusive change in the ³¹P{¹H} NMR spectra of complex **A** was observed when temperature was raised from 298 K to 400 K (Fig. S31). The color of sample remained same (dark blue) upon cooling the sample back to 298 K.

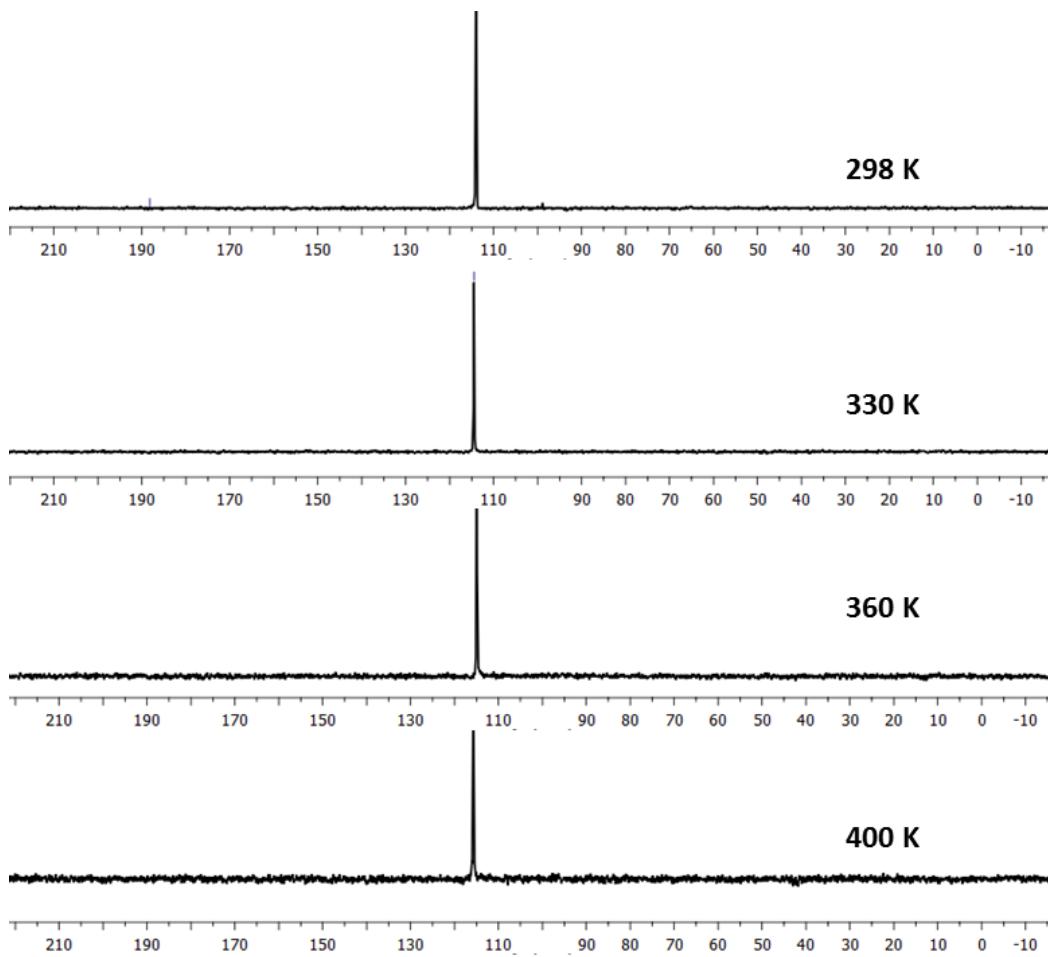


Fig. S41. Variable temperature $^{31}\text{P}\{\text{H}\}$ NMR (202.44 MHz, DMSO-d₆) spectra for complex **A**.

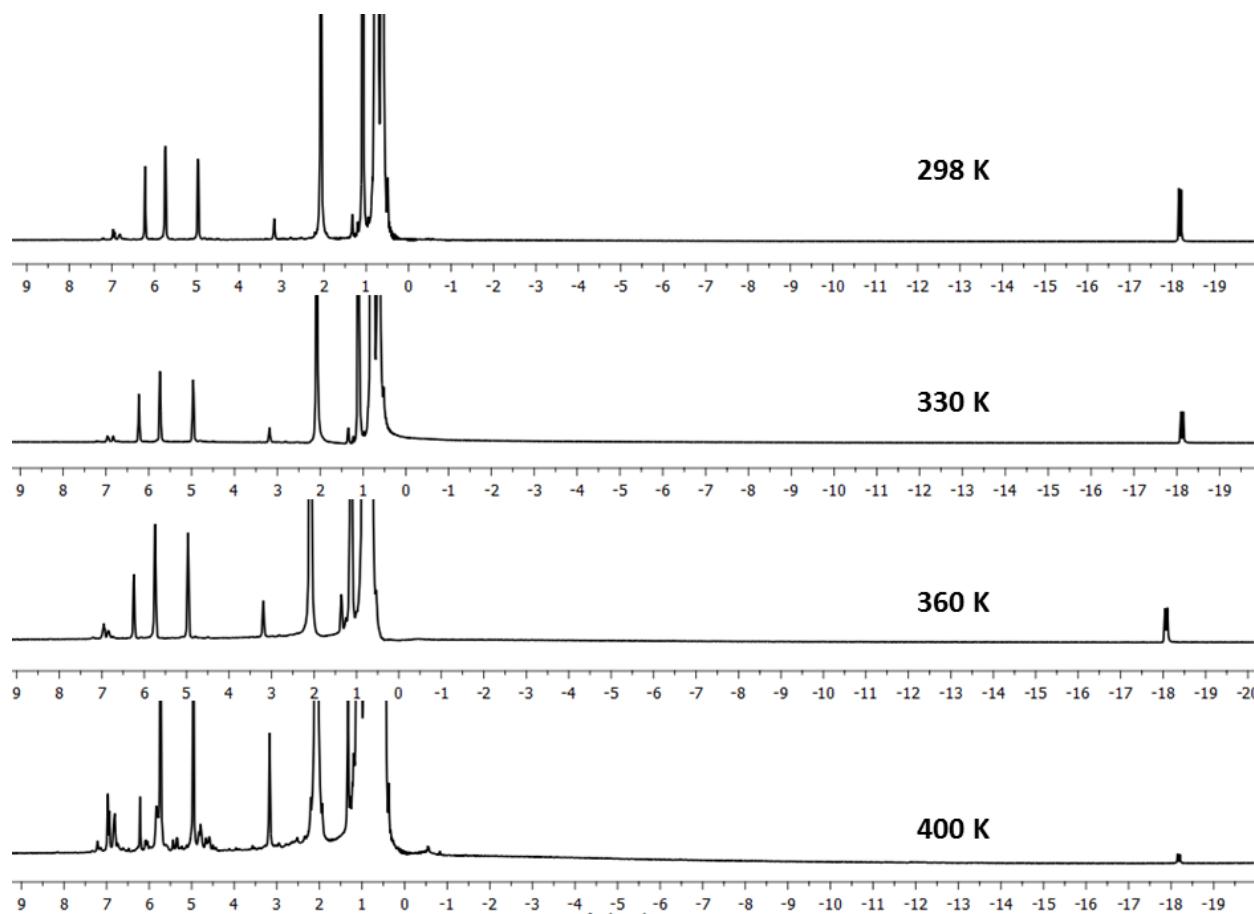
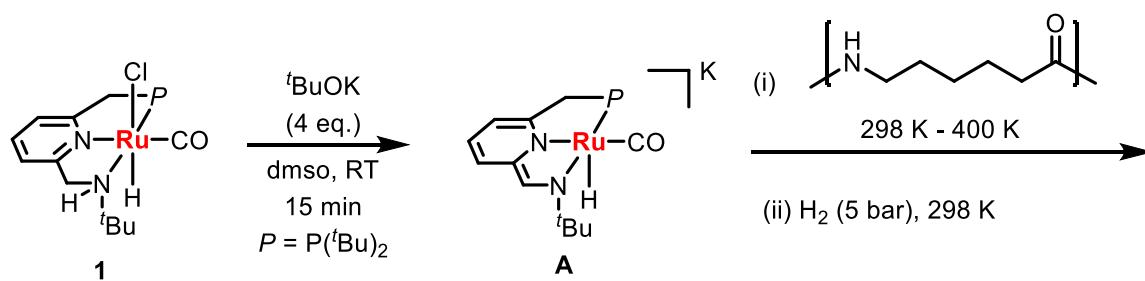


Fig. S42. Variable temperature ^1H NMR (500 MHz, DMSO-d₆) spectra for complex **A**.

14.3. Reactivity of nylon 6 with complex 1 and KO^tBu in DMSO



In a glovebox, complex **1** (19.5 mg, 0.04 mmol) and KO*t*Bu (~18 mg, 0.16 mmol) were suspended in DMSO-d6 (0.5 mL). The resulting red solution was transferred to a J. Young valve NMR tube. After 15 minutes the color of the solution turned to dark blue and the NMR spectra showed the clean formation of complex **A**. Nylon 6 (powder, Mw ~11000, 20 mg, 0.18 mmol of the monomer) was added to the NMR tube and the reaction was studied by variable temperature (298 K – 400 K) NMR spectroscopy. No significant change was observed in the ¹H and ³¹P {¹H} NMR spectra till 360 K. Interestingly, at 400 K the hydride signal completely disappeared in the ¹H NMR spectrum, and the ³¹P {¹H} NMR spectrum showed the formation of a mixture of complexes (Fig.s S33-34). Similar ¹H and ³¹P {¹H} NMR spectra were observed when the sample was cooled back to 298 K. Interestingly, the color of the sample in this process changed to dark red from dark blue, which is different from when only complex **A** was heated in DMSO (section 12.2).

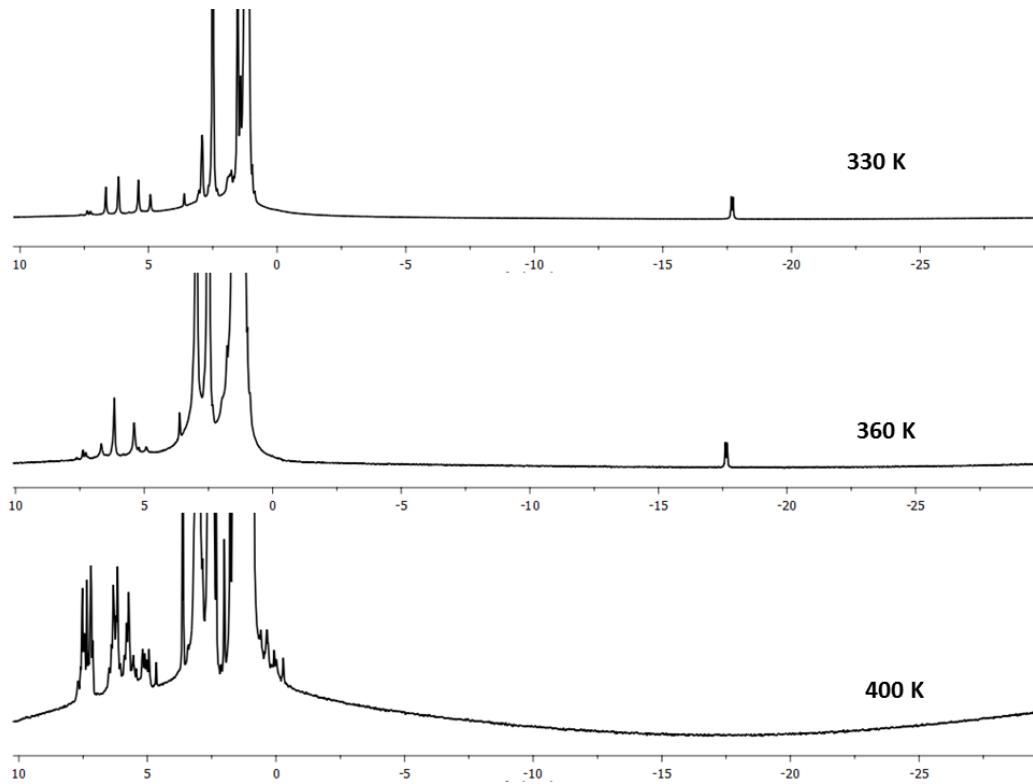


Fig. S43. Variable temperature ¹H NMR (400.36 MHz, DMSO-d6) spectra for reaction of nylon 6 with complex **A**.

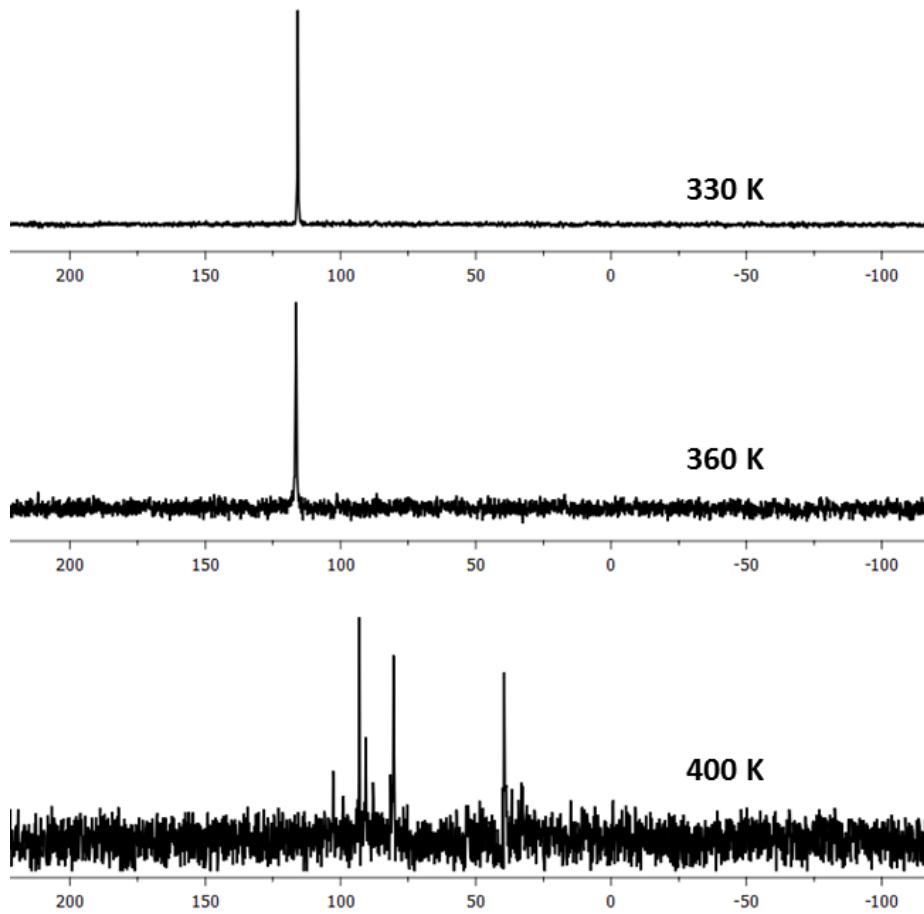


Fig. S44. Variable temperature $^{31}\text{P}\{\text{H}\}$ NMR (162.08 MHz, DMSO-d6) spectra for reaction of nylon 6 with complex **A**.

Addition of H₂ (5 bar) to the same NMR tube at 298 K resulted in the observation of multiple ruthenium hydride species in the ^1H NMR spectrum, featured by broad signals at δ -5.56, -5.78, -10.30 and -11.34. The signals at δ -5.56, -5.78 fit well with a ruthenium *trans* dihydride complex **C** that was independently prepared by the reaction of complex **1** with KO^tBu and H₂ (hydride signals at δ -4.73 and -5.12 in THF-d8 and at δ -5.23 and -5.42 in DMSO-d6). The $^{31}\text{P}\{\text{H}\}$ NMR spectrum of the reaction mixture after addition of H₂ also showed a mixture of complexes and

contain a signal at δ 123.9, very close to that of complex **C** (δ 123.5 in THF-d8, δ 122.93 in DMSO-d6).

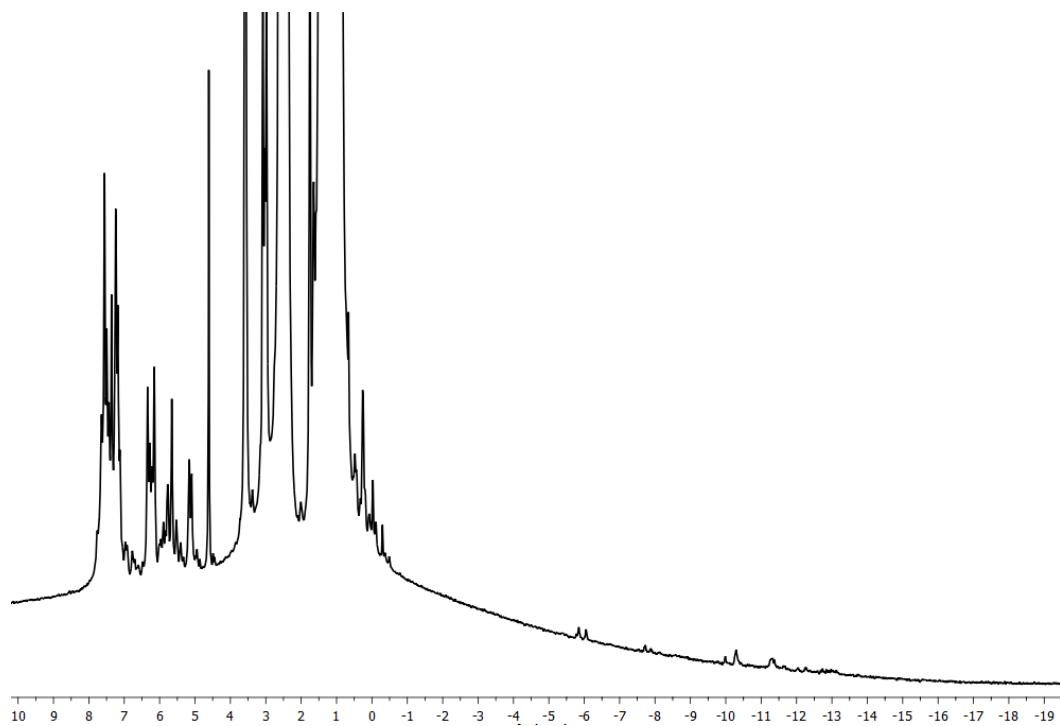


Fig. S45. ^1H NMR (500.08 MHz, DMSO-d6, 298 K) spectrum after adding H_2 (5 bar, 5 minutes, 298 K) to the reaction of nylon 6 with complex **A**.

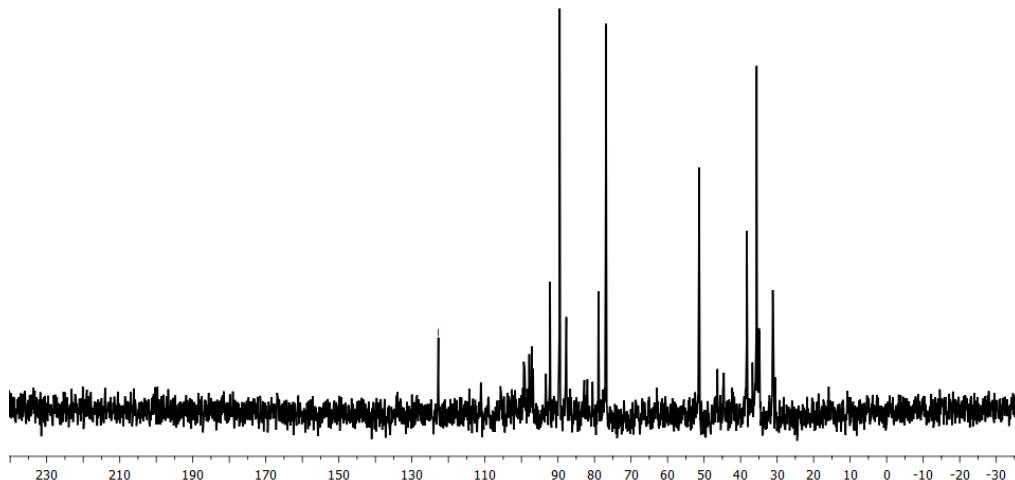
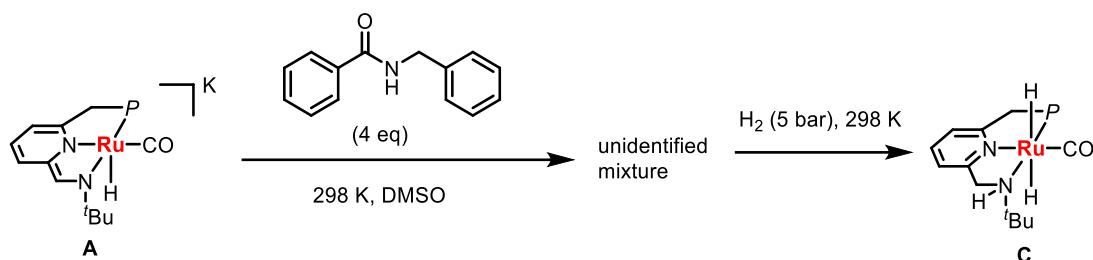


Fig. S46. $^{31}\text{P}\{\text{H}\}$ NMR (202 MHz, DMSO-d6, 298 K) spectrum after adding H_2 (5 bar, 5 minutes, 298 K) to the reaction of nylon 6 with complex **A**.

14.4. Reactivity of N-benzylbenzamide with complex 1 / KO^tBu in DMSO



In a glovebox, complex **1** (19.5 mg, 0.04 mmol) and KO^tBu (~18 mg, 0.16 mmol) were suspended in DMSO-d6 (0.5 mL). The resulting red solution was transferred to a J. Young valve NMR tube. After 15 minutes the color of the solution turned to dark blue and the NMR spectra showed the clean formation of complex **A**. N-benzylbenzamide (34 mg, 0.16 mmol) was added to the NMR tube and the reaction was studied by NMR spectroscopy. ¹H NMR spectrum taken after 5 minutes of addition of N-benzylbenzamide showed disappearance of the hydride signals and the ³¹P{¹H} NMR spectrum showed the formation of mixture of complexes (Fig.s S37 II and S38 II). Interestingly, addition of hydrogen gas (5 bar) to the same NMR tube at room temperature resulted in the formation of ruthenium *trans* dihydride complex **C** (Fig.s S37 III-IV and S38 III-IV). Heating the same reaction mixture at 110 °C for 24 hours resulted in the formation of benzyl amine and benzyl alcohol as detected by the GC.

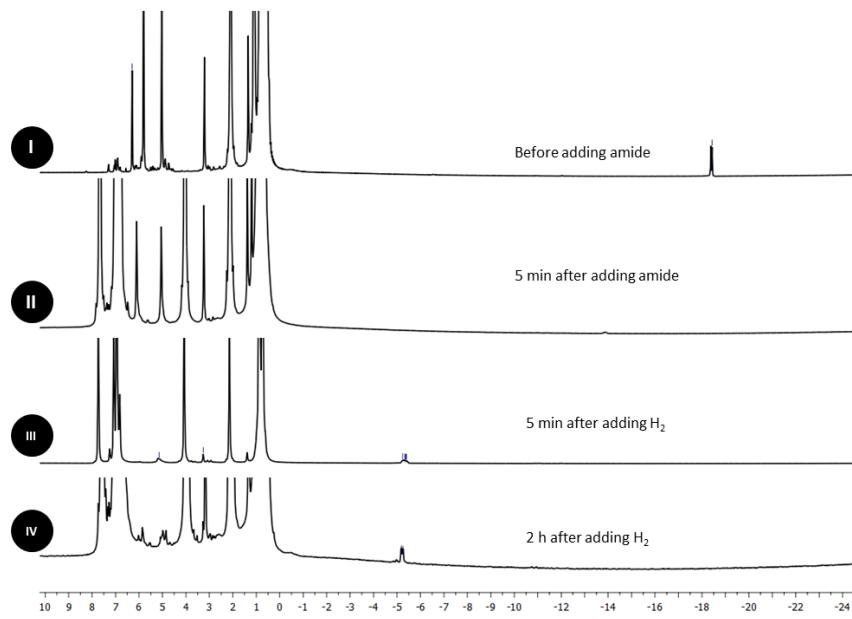


Fig. S47. ^1H NMR (500.08 MHz, DMSO-d6, 298 K) spectrum for the formation of complex **A** (I); ^1H NMR spectrum taken after 5 minutes of addition of N-benzylbenzamide to **A** (II); ^1H NMR spectrum taken after 5 minutes of addition of H_2 to the reaction mixture obtained from step no II (III); ^1H NMR spectrum taken after 2 h of addition of H_2 (IV).

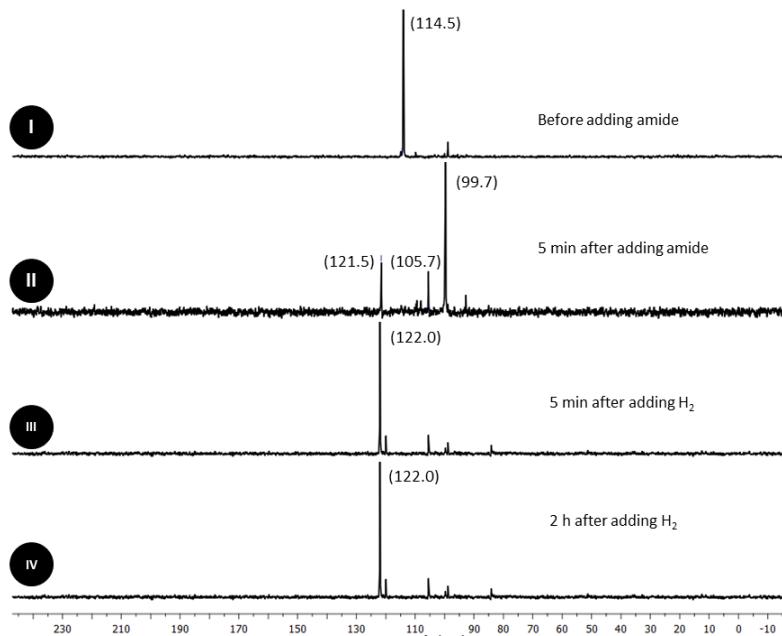
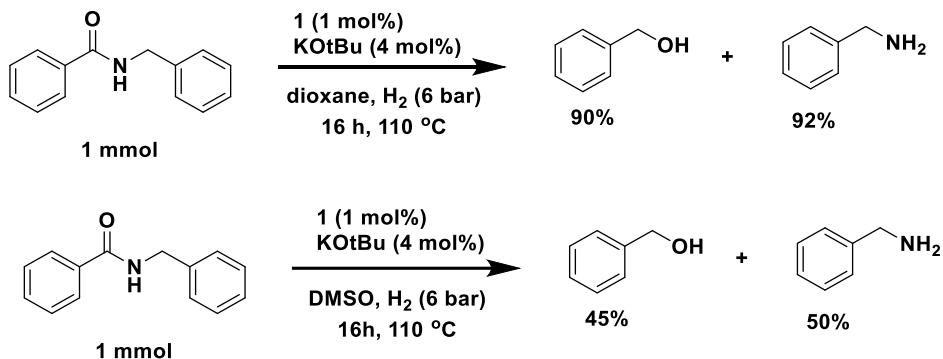
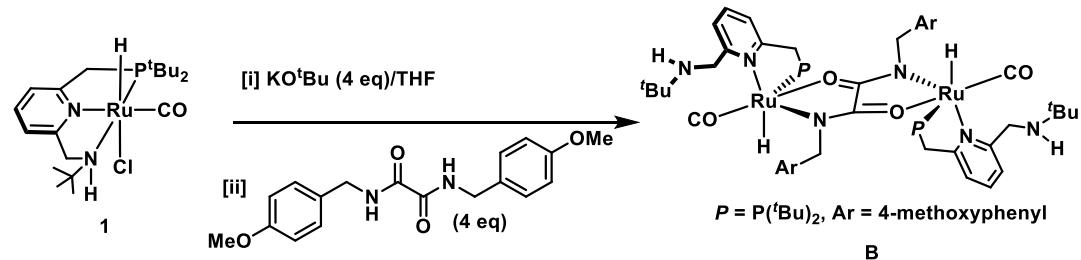


Fig. S48. $^{31}\text{P}\{\text{H}\}$ NMR (202 MHz, DMSO-d6, 298 K) spectrum for the formation of complex **A** (I); $^{31}\text{P}\{\text{H}\}$ NMR spectrum taken after 5 minutes of addition of N-benzylbenzamide to **A** (II); $^{31}\text{P}\{\text{H}\}$ NMR spectrum taken after 5 minutes of addition of H_2 to the reaction mixture obtained from step no II (III); $^{31}\text{P}\{\text{H}\}$ NMR spectrum taken after 2 h of addition of H_2 (IV).

We also studied the catalytic hydrogenation of N-benzylbenzamide (1 mmol) using the combination of complex **1** (5 mg, 0.01 mmol) and KO^tBu (4.5 mg, 0.04 mmol) in DMSO or 1,4-dioxane (2 mL) under 6 bar H₂ pressure at 110 °C for 16 h. Analysis of the reaction mixture by the GC showed higher yield of the hydrogenated products benzyl alcohol and benzyl amine in 1,4-dioxane than in DMSO (see below).



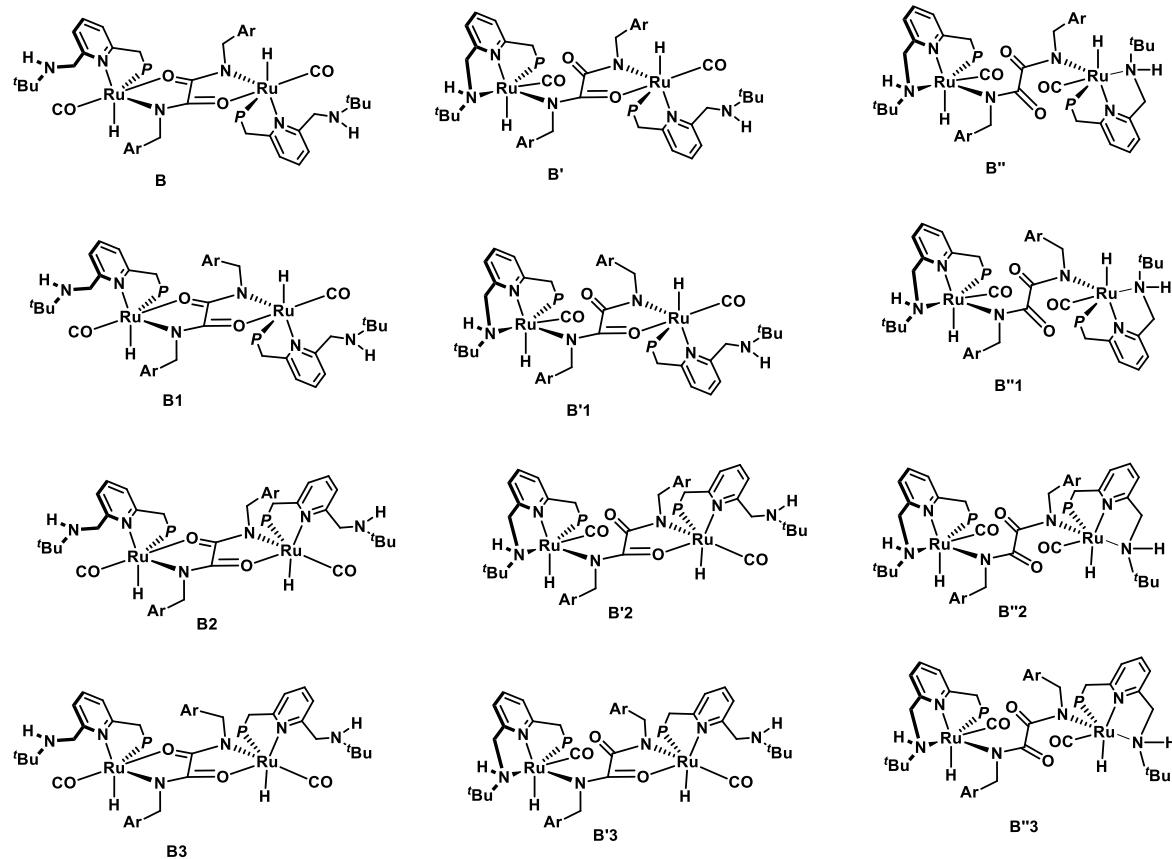
14.5. Reactivity of N1,N2-bis(4-methoxybenzyl)oxalamide with complex 1/KOtBu in THF or DMSO



In a glovebox, **1** (39 mg, 0.08 mmol) and KO^tBu (~36 mg, 0.32 mmol) were suspended in THF (0.7 mL). The resulting red solution was transferred to a J. Young valve NMR tube. After 15 min the color of the solution turned to dark blue and the NMR spectra showed clean formation of complex **A**. N1,N2-bis(4-methoxybenzyl)oxalamide (104 mg, 0.32 mmol) was added to the NMR tube and the reaction was studied at 298 K by NMR spectroscopy. ³¹P{¹H} NMR spectroscopy showed the formation of multiple species with one major complex (δ 101.4). The NMR spectrum remained the same up to 24 hours after which the

resulting reaction mixture in THF was filtered, layered with pentane and kept for 48 h at -30 °C, resulting in formation of a yellow crystalline precipitate. X-ray diffraction of a single crystal of this precipitate revealed the structure of the final product as **B**. However, the NMR spectra of the crystalline material in toluene-d₈ (obtained separately from another reaction using the same procedure) showed a mixture of species as evident by the five hydride signals in the ¹H NMR spectrum (δ – 13.3 ($^2J_{HP}$ = 17.6 Hz), -13.67 ($^2J_{HP}$ = 17.6 Hz), -14.16 ($^2J_{HP}$ = 17.6 Hz), -14.35 ($^2J_{HP}$ = 17.6 Hz) and -16.06 ($^2J_{HP}$ = 19.5 Hz)) and signals in the ³¹P{¹H} NMR spectrum at (δ 101.5, 102.3, 102.6, 103.3, 104.8). We were unable to get clean spectra of the complex **B**, which could be because of the presence of isomers of **B** due to its molecular dynamics.

Possible isomers of complex **B** ($P = P^tBu_2$, Ar = 4-methoxyphenyl)



DOSY NMR study

The same sample was also analysed by the Diffusion NMR spectroscopy in toluene-d₈ (500 MHz). The diffusion coefficients were calculated using the hydride signals and the signals corresponding to the solvent. The diffusion coefficient obtained from each hydride signals (Fig. S39) corresponding to **B** (and its isomers presumably) were found to be the same and 2.4 times stronger than that of **1**. This is in agreement with the actual comparison of molecular weight (Mol wt of **B**/Mol wt of **1** = 2.4).

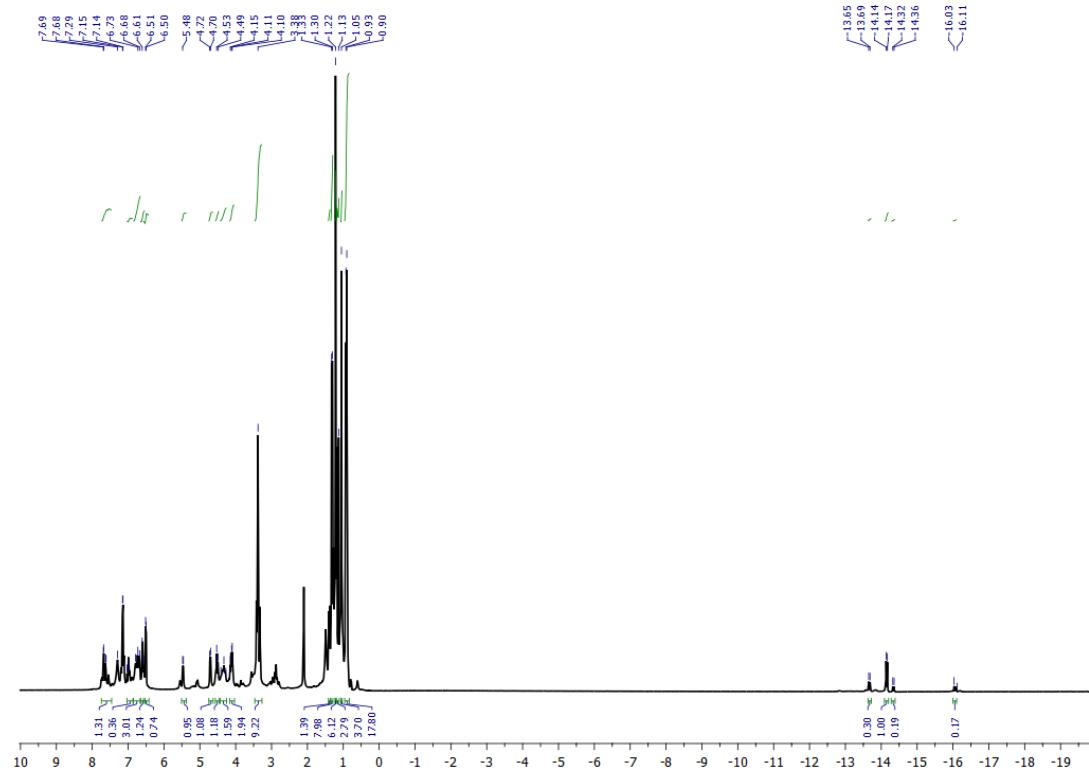


Fig. S49. ^1H NMR (500 MHz, toluene-d8, 298 K) spectrum corresponding to the formation of complex **B**.

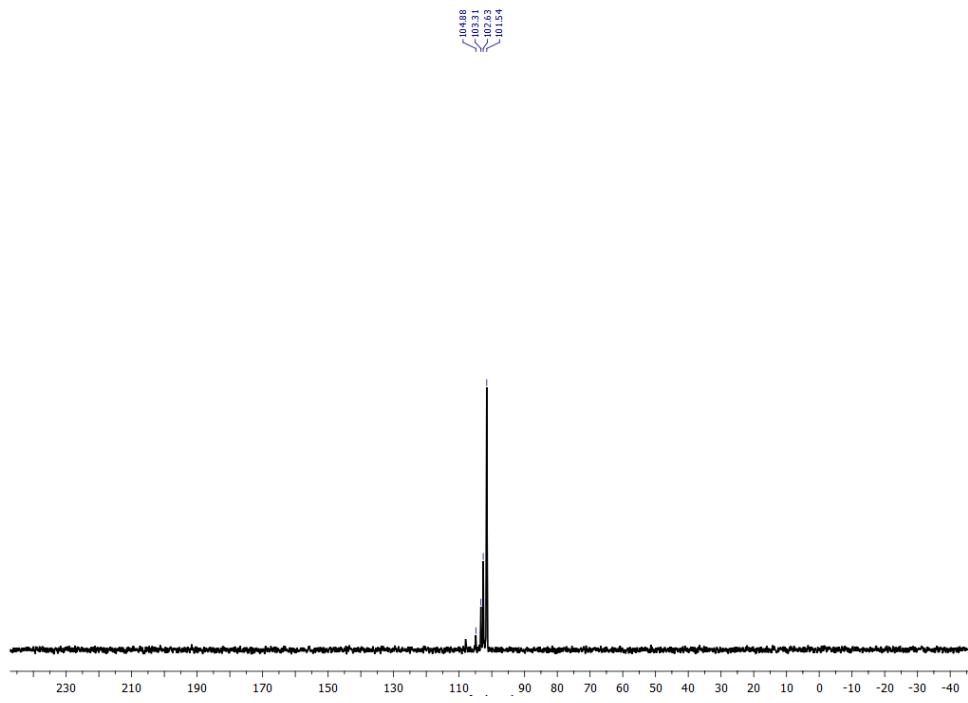


Fig. S50. $^{31}\text{P}\{\text{H}\}$ NMR (202 MHz, toluene-d8, 298 K) spectrum corresponding to the formation of complex **B**.

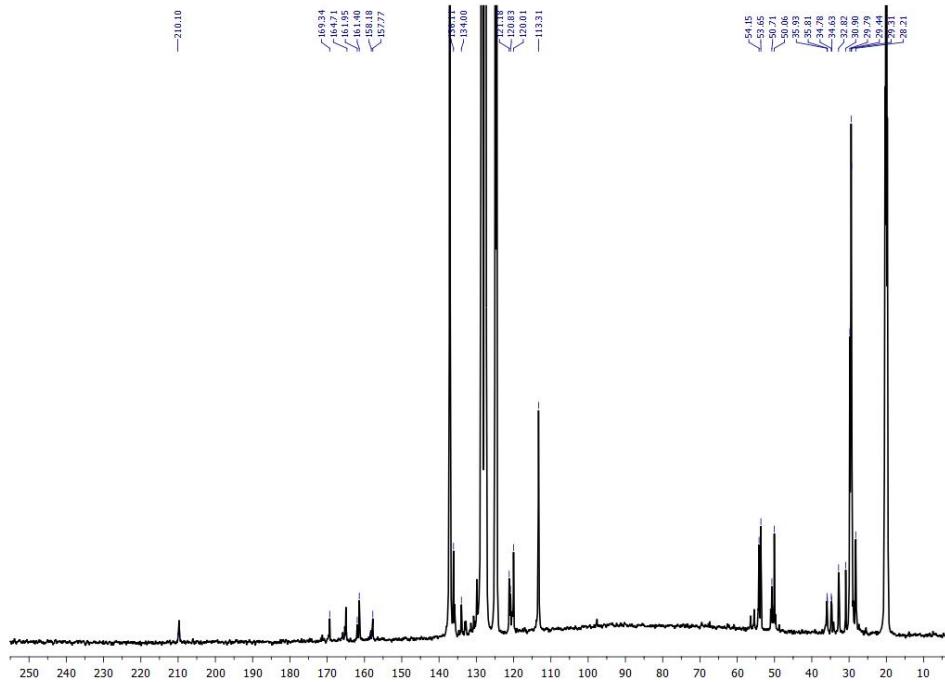


Fig. S51. $^{13}\text{C}\{\text{H}\}$ NMR (125.75 MHz, toluene-d8, 298 K) spectrum corresponding to the formation of complex **B**.

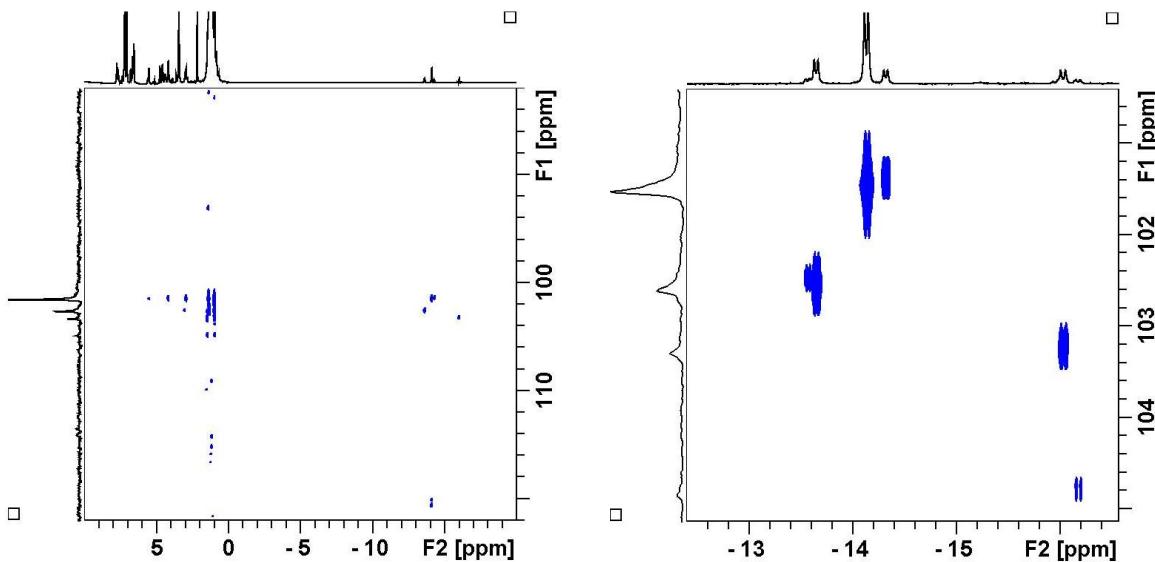


Fig. S52. $^1\text{H}\{^{31}\text{P}\}$ HMBC NMR (500 MHz, toluene-d8, 298 K) spectrum for the formation of complex **B**; the selected hydride region correlating with the phosphine signals is shown on the right.

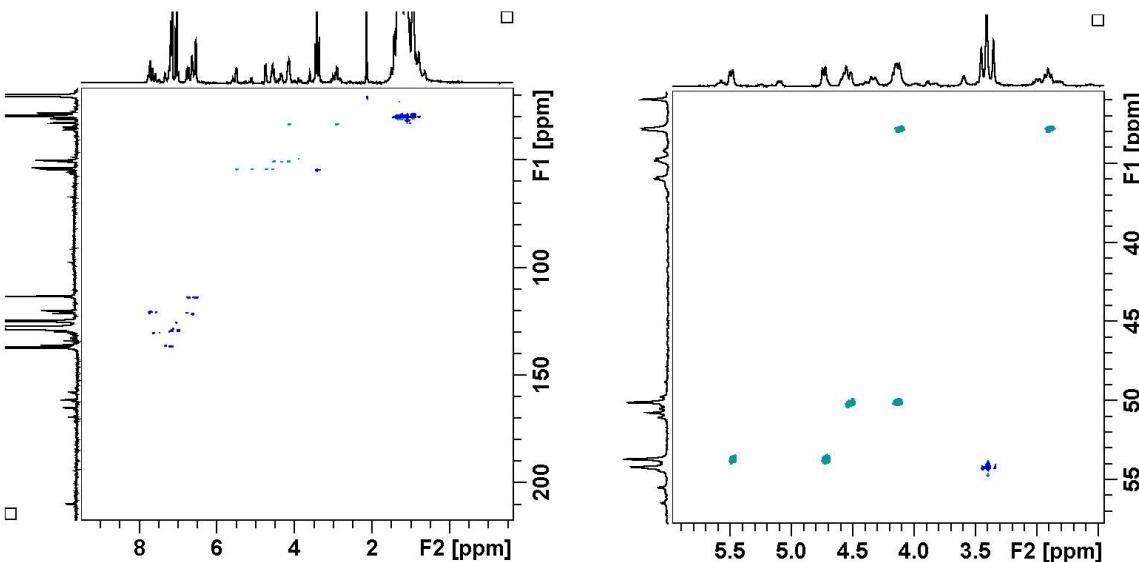


Fig. S53. $^1\text{H}\{^{13}\text{C}\}$ HSQC NMR (500 MHz, toluene-d8, 298 K) spectrum for the formation of complex **B**.

$^1\text{H}\{^{15}\text{N}\}$ HMBC NMR study:

In order to distinguish between the coordinated and uncoordinated amine sidearm of the pincer complexes (isomers of **B**) we carried $^1\text{H}\{^{15}\text{N}\}$ HMBC NMR study. ^{15}N NMR chemical shift corresponding to the N^tBuH group of the isomers of complex

B were found to be at δ 59.03, 60.87, 61.36, 62.38 and 63.73 (Fig. S44). To make a suitable comparison we carried the $^1\text{H}\{^{15}\text{N}\}$ HMBC NMR study of complex **1** which contains the PNNH pincer ligand coordinated to ruthenium and of the corresponding free PNNH pincer ligand. ^{15}N NMR chemical shift corresponding to the N^tBuH group of the free PNNH pincer ligand was found to be at 60.0 and that corresponding to complex **1** was found to be at 59.2 (Fig. S45). As the ^{15}N NMR chemical shifts corresponding to the free and bound N^tBuH group of the PNNH pincer ligand were too close, we were unable to distinguish between the free and the coordinated amine side arms among the isomers of complex **1** by the $^1\text{H}\{^{15}\text{N}\}$ HMBC NMR study.

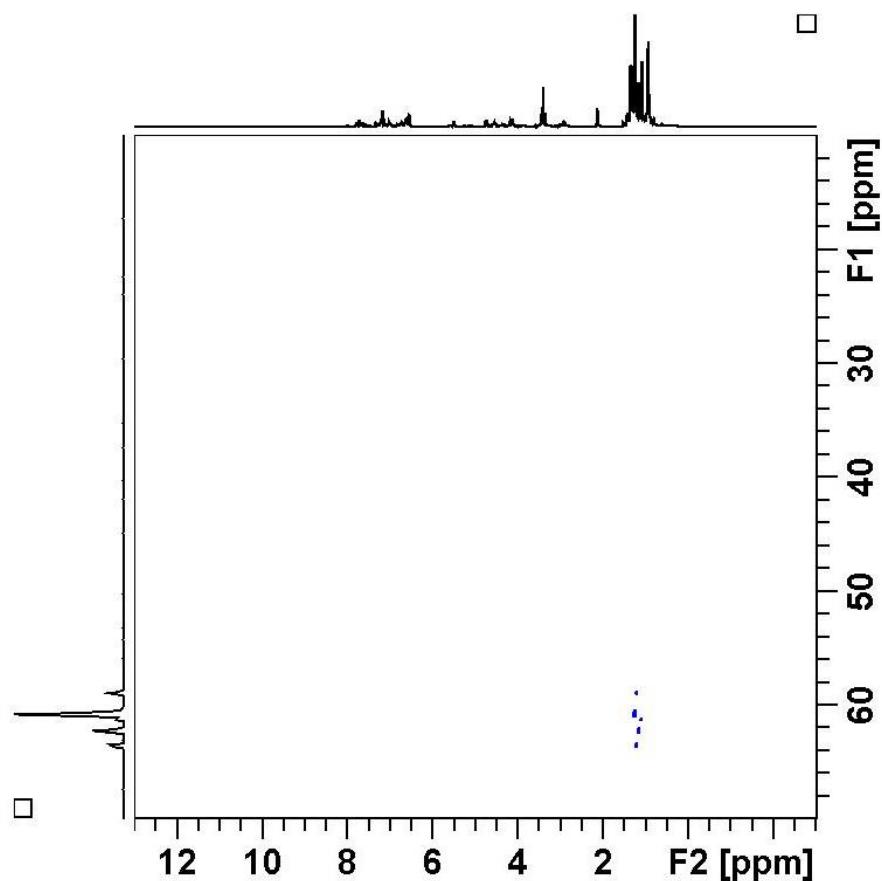


Fig. S54. $^1\text{H}\{^{15}\text{N}\}$ HMBC NMR (298 K, toluene-d8) for the formation of complex **B**.

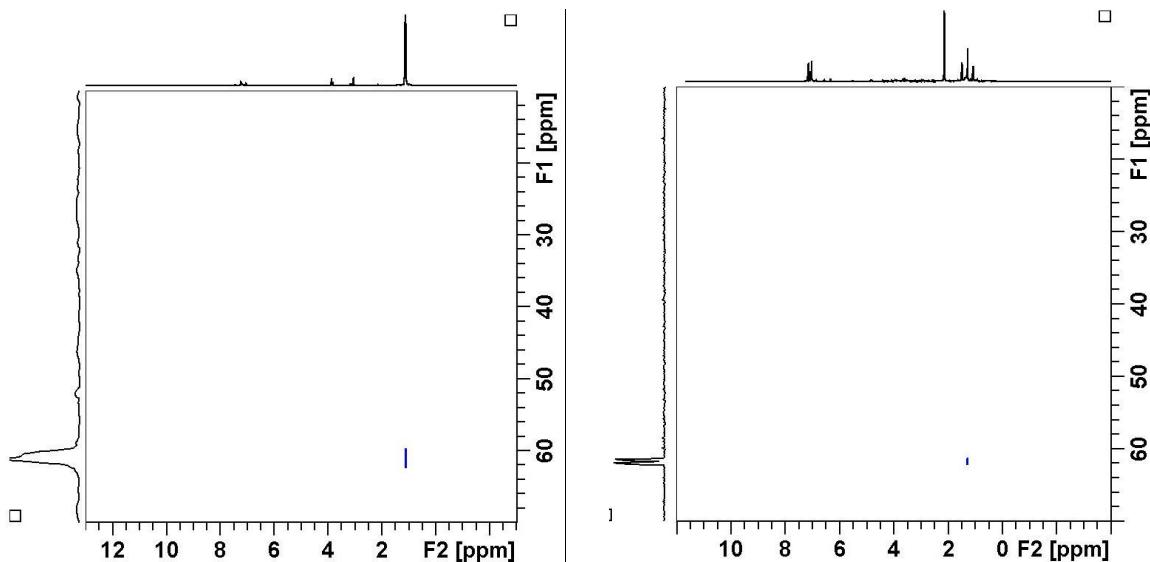


Fig. S55. $^1\text{H}\{^{15}\text{N}\}$ HMBC NMR (298 K, toluene-d8) for the free PNNH pincer ligand (left) and the bound PNNH pincer ligand complex **1** (right).

15. Crystallographic details

The diffraction data of complex **B** was collected on Rigaku XtaLAB diffractometer, CuK α ($\lambda=1.54184 \text{ \AA}$), graphite monochromator, $-29 \leq h \leq 30$, $-14 \leq k \leq 16$, $-46 \leq l \leq 46$, frame scan width = 0.5° , 55763 reflections collected, 12314 independent reflections ($R\text{-int}=0.0389$). The data were processed with CrysAlisPro 1.171.38.41 (Rigaku OD, 2015). Structure solved with SHELXT program. Full matrix least-squares refinement based on F^2 with SHELXL-2014/7 on 746 parameters with 0 restraints gave final $R_1=0.0405$ (based on F^2) for data with $|l| > 2\sigma(l)$ and, $R_1=0.0439$ on 12314 reflections, goodness-of-fit on $F^2 = 1.100$, largest electron density peak $1.170 \text{ e} \cdot \text{\AA}^{-3}$. Largest hole $-0.380 \text{ e} \cdot \text{\AA}^{-3}$. Platon/Squeeze procedure was used to remove electron density peaks of disordered solvent molecule (THF) during refinement.

Table S8. Crystallographic details for complex **B**

Formula	C ₅₈ H ₉₀ N ₆ O ₆ P ₂ Ru ₂ , C ₅ H ₁₂ [+solvent (THF)]
Formula weight (g mol ⁻¹)	1303.58*
Crystal system	monoclinic
Space group	I 2/a
Crystal size (mm)	0.121 x 0.029 x 0.018
Crystal color and shape	pale yellow prism
Temperature (K)	100(2)
Wavelength (Å)	1.54184
a (Å)	25.583(5)
b (Å)	14.101(3)
c (Å)	38.615(8)
α (°)	90(-)
β (°)	104.83(3)
γ (°)	90(-)
Volume (Å ³)	13466(5)
Z	8
ρ _{calc} (g cm ⁻³)	1.286*
μ (mm ⁻¹)	4.477*
No. of unique reflections	12314
R _{int}	0.0389
Completeness (%) to Θ (°)	99.9 to 68.250
Data / restraints / parameters	12314 / 0 / 746
Goodness-of-fit on F ²	1.100
Final R1 and wR2 indices [<i>I</i> > 2σ(<i>I</i>)]	0.0405 ; 0.1056
R1 and wR2 indices (all data)	0.0439 ; 0.1083

*calculated without taking into account additional solvent (THF) molecule.

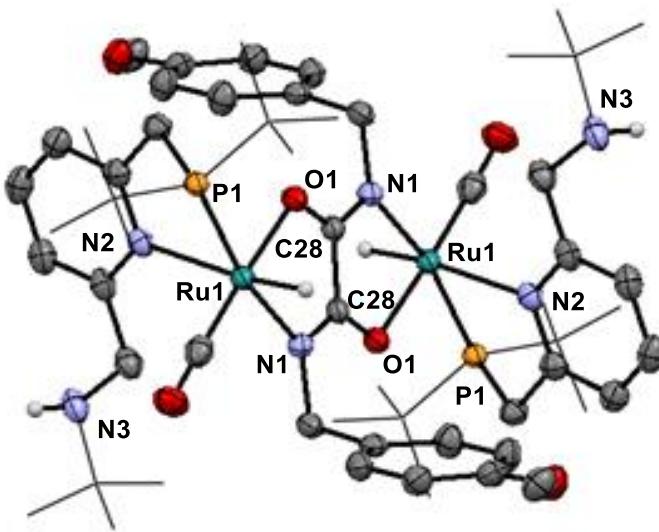


Fig. S56. Single crystal X-ray structure of **B** with thermal ellipsoid at 50% probability level, hydrogen atoms except the Ru-H are omitted for clarity. Selected bond lengths in Å: Ru1O1 2.1599(19), Ru1N1 2.135(2), Ru1P1 2.2892(8), Ru1N2 2.340(3), N1C28 1.301(4), O1C28 1.280(3).

16. DFT Calculations

All geometries were optimized using Truhlar's M06-L functional,¹¹ the triple- ξ def2-TZVP basis set¹² and W06 density fitting to increase computational efficiency¹³ as well as Grimme's empirical GD3 dispersion correction.¹⁴ Frequency calculations at this level of theory were run at 423.15 K and 69.08 atm in order to confirm stationary points and transition states, as well as to compute thermodynamic properties. Single point energies of the optimized structures were computed using the range-separated meta-GGA hybrid functional ω B97M-V of the Head-Gordon group¹⁵ including dispersion correction (DFT-NL);¹⁶ which was recently shown to give excellent results on a thermochemical benchmark set of metal organic reactions¹⁷ together with the triple- ξ def2-TZVPP basis set¹² and the corresponding auxiliary basis sets, def2/J¹³ and def2-TZVPP/C,¹⁸ for RIJCOSX density fitting. Gibbs Free Energies were computed following Neese and co-workers' approach¹⁹ by adding the Free Energy correction terms from the

frequency calculations to the single point energies at the ω B97M-V/def2-TZVPP level of theory in the solution phase (DMSO), using the integral equation formalism variant (IEFPCM) in the SMD variation of Truhlar and co-workers,²⁰ according to

$$G_{SMD}^{\omega B97M-V} = E_{el/SMD}^{\omega B97M-V} + cor_{freq/gas}^{M06-L}$$

Optimizations and frequency calculations were done using the Gaussian 16 software suite in the B.01 revision (Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016). Single point energy calculations were performed using the ORCA Software package in the 4.2.1 release.²¹

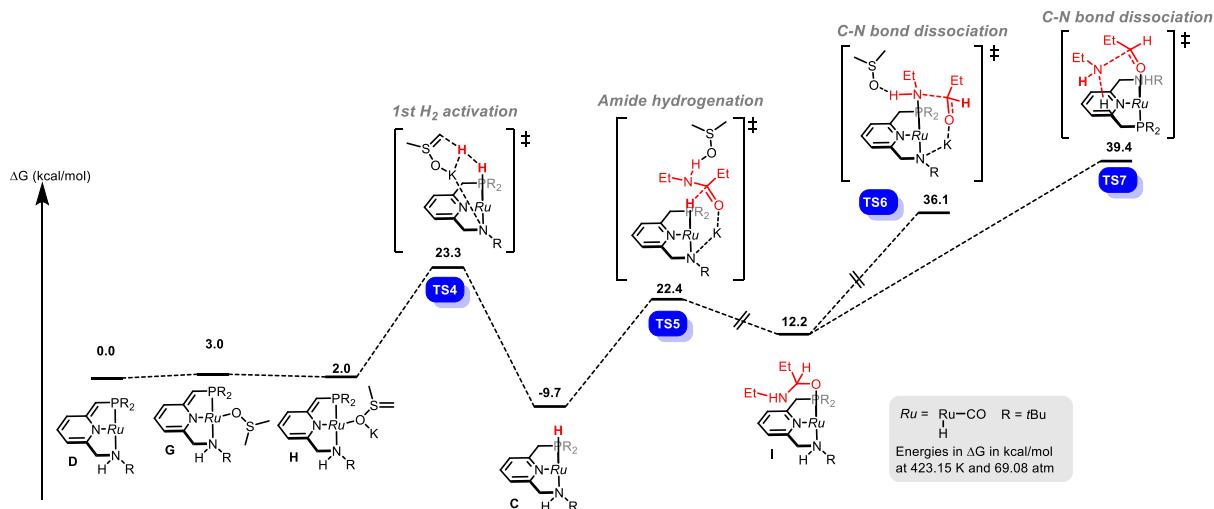


Fig. S57. Additional DFT calculations to probe the possible involvement of DMSO-enolate stabilized intermediates and transition states. Values correspond to Gibbs free energies with respect to the starting material in kcal/mol calculated at 423.15 K and 69.08 atm in the gas phase and in solution (DMSO, values in brackets).

Discussion

As observed experimentally, addition of DMSO to the dearomatized complex is energetically unfavored (Fig. S57). Importantly, the strong base DMSOK, that might be formed during the reaction conditions, is not able to accelerate H₂-splitting (**TS4** compared to **TS1A** or **TS1B** in Scheme 2 of the manuscript). On the other hand, potassium as a Lewis acid and DMSO as a H-bond acceptor might slightly facilitate the amide hydrogenation step (**TS5**, 22.4 kcal/mol). In the case of C–N cleavage (**TS6**, 36.1 kcal/mol) this effect seems to be insufficient to allow for facile hemiaminal dissociation. We also probed the involvement of the P-arm for the C–N bond dissociation from the alkoxide intermediate **I**, but the barrier was significantly higher (**TS7**, 39.4 kcal/mol) compared to the N-arm (Scheme 2 of the manuscript, **TS3A**). For the involvement of the N-H group, no transition state could be located. We thus performed surface scans in the absence (Fig. S58) and presence of DMSOK (Fig. S59). Indeed, no discernable transition state is observed on the PES slice. This situation might change in the presence of a H-bonding network and we regard **TS3A** (Scheme 2, manuscript) thus as an upper limit for the catalyzed C–N bond scission. Similar observations are made in for the

potassium salt of the hemiaminal (Fig. S60). Again, a H-bonding network is thought to highly stabilize the leaving amido unite to give an overall exergonic reaction, together with the appearance of a transition state. Further studies in that direction are ongoing.

Surface scans

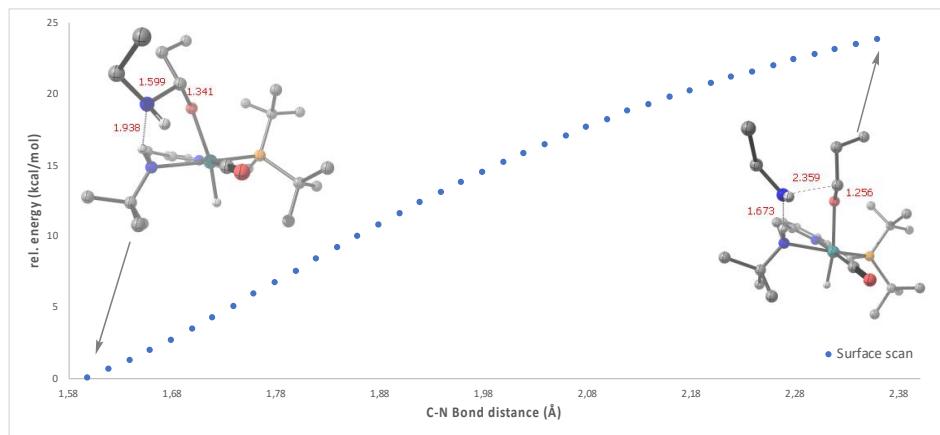


Fig. S58 Surface scan for the C–N bond dissociation starting from the O-bound alkoxide intermediate. C–H bonds omitted for clarity.

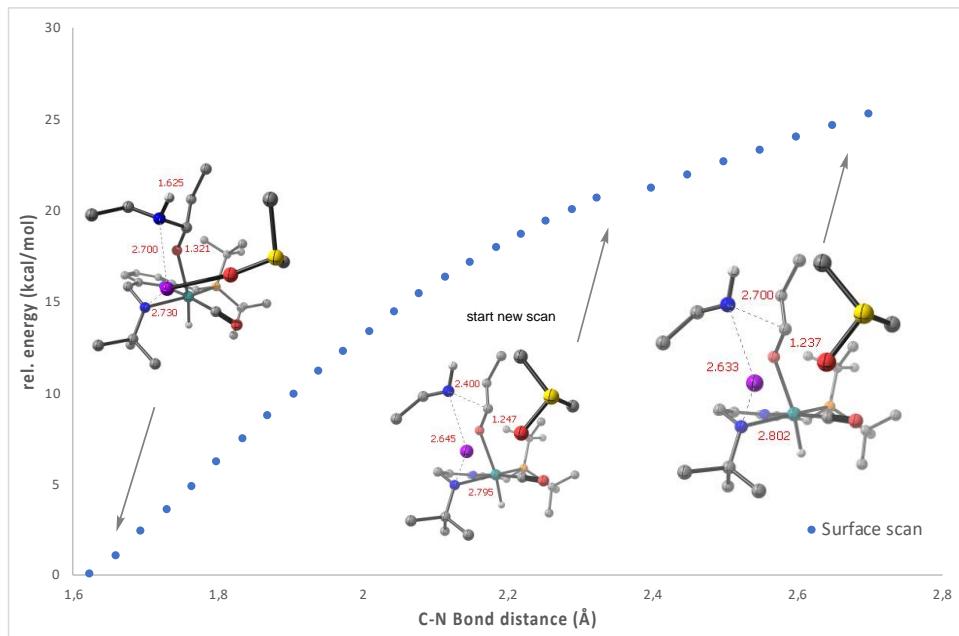


Fig. S59 Surface scan for the C–N bond dissociation starting from the O-bound alkoxide intermediate in the presence of DMSOK after proton transfer from the ligand NH site to the DMSO enolate. C–H bonds omitted for clarity.

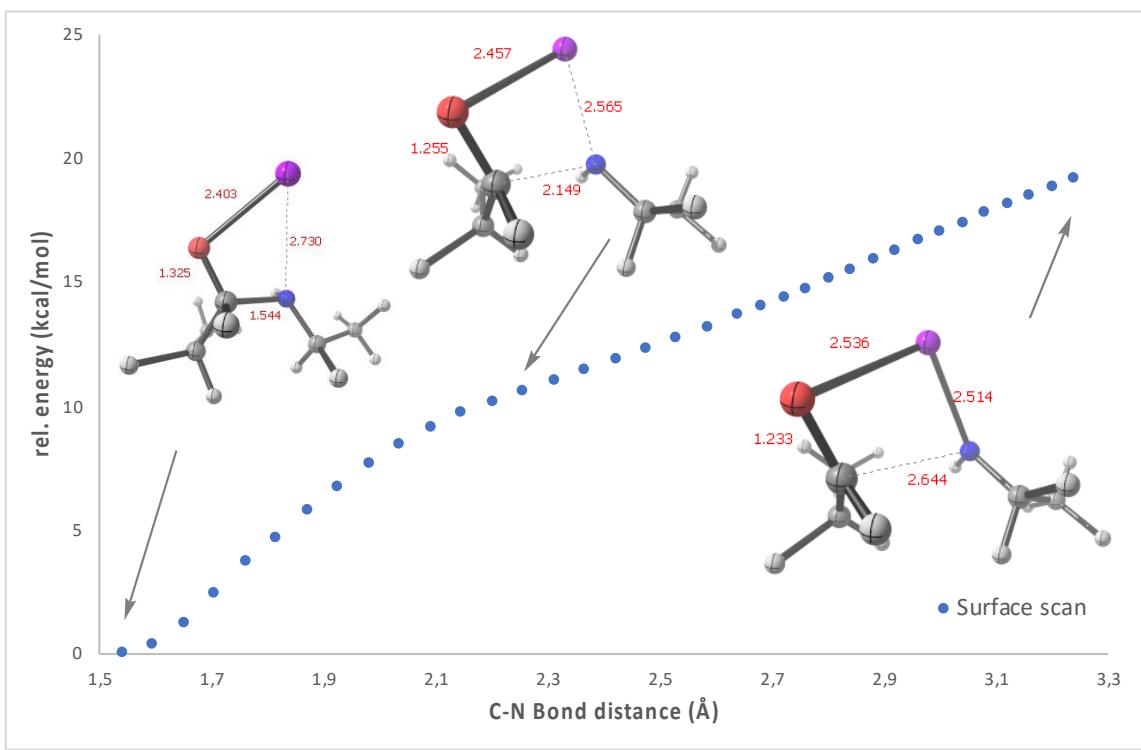


Fig. S60 Surface scan for the C–N bond dissociation starting from the potassium salt of the hemiaminal.

17. References

1. Gnanaprakasam, B.; Balaraman, E.; Gunanathan, C.; Milstein, D. Synthesis of Polyamides from Diols and Diamines with Liberation of H₂. *J. Polym. Sci. A: Polym. Chem.*, **2012**, *50*, 1755-1765.
2. Fogler, E.; Garg, J. A.; Hu, P.; Leitus, G.; Shimon, L. J. W.; Milstein, D. System with Potential Dual Modes of Metal–Ligand Cooperation: Highly Catalytically Active Pyridine-Based PNNH–Ru Pincer Complexes. *Chem. Eur. J.*, **2014**, *20*, 15727-15731.
3. Kumar, A.; Janes, T.; Espinosa-Jalapa, N. A.; Milstein, D. Selective Hydrogenation of Cyclic Imides to Diols and Amines and Its Application in the Development of a Liquid Organic Hydrogen Carrier. *J. Am. Chem. Soc.*, **2018**, *140*, 7453-7457.

4. Balaraman, E.; Gnanaprakasam, B.; Shimon, L. J. W.; Milstein, D. Direct Hydrogenation of Amides to Alcohols and Amines under Mild Conditions. *J. Am. Chem. Soc.*, **2010**, *132*, 16756-16758.
5. Zhang, J.; Leitus, G.; Ben-David, Y.; Milstein, D. Facile Conversion of Alcohols into Esters and Dihydrogen Catalyzed by New Ruthenium Complexes. *J. Am. Chem. Soc.*, **2005**, *127*, 10840-10841.
6. Gunanathan, C.; Milstein, D. Selective Synthesis of Primary Amines Directly from Alcohols and Ammonia. *Angew. Chem. Int. Ed.*, **2008**, *47*, 8661-8664.
7. Han, Z.; Rong, L.; Wu, J.; Zhang, L.; Wang, Z.; Ding, K. Catalytic Hydrogenation of Cyclic Carbonates: A Practical Approach from CO₂ and Epoxides to Methanol and Diols. *Angew. Chem., Int. Ed.*, **2012**, *51*, 13041 -13045.
8. Sharma, B.; Ubags, L.; Keul, H.; Höcker, H.; Loontjens T.; van Benthem, R. Synthesis and characterization of alternating poly(amide urethane)s from ε-caprolactam, amino alcohols, and diphenyl carbonate. *Polymer*, 2004, **45**, 5427–5440.
9. Chen, J.; Wang, J.; Tu, T. Ruthenium-Pincer-Catalyzed Hydrogenation of Lactams to Amino Alcohols. *Chem. Asian J.*, **2018**, *13*, 2559 –2565.
10. Neira-Velasquez, M. G.; Rodriguez-Hernandez, M. T.; Hernandez-Hernandez, E.; Ruiz-Martinez, A. in *Handbook of Polymer Synthesis, Characterization, and Processing*, ed. E. Saldivar-Guerra and E. Vivaldo-Lima, John Wiley & Sons, Inc, **2013**, 355-366.
11. Zhao, Y.; Truhler, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.*, **2006**, *125*, 194101.
12. Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297-3305.
13. Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.

14. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.*, **2010**, *132*, 154104.
15. Mardirossian, N.; Head-Gordon, M. *J. Chem. Phys.*, **2016**, *144*, 214110.
16. (a) Vydrov, O. A.; Voorhis, T. V. Nonlocal van der Waals density functional: The simpler the better. *J. Chem. Phys.* **2010**, *133*, 244103. (b) Hujo, W.; Grimme, S. Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. *J. Chem. Theory Comput.*, **2011**, *7*, 3866-3871.
17. Iron, M. A.; Janes, T. Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange–Correlation Functionals: The MOBH35 Benchmark Database. *J. Phys. Chem. A*, **2019**, *123*, 3761-3781.
18. Hellweg, A.; Hattig, C.; Hoefener, S.; Klopper, W. Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. *Theor Chem Acc*, **2007**, *117*, 587–597.
19. Mondal, B.; Neese, F.; Ye, S. Control in the Rate-Determining Step Provides a Promising Strategy to Develop New Catalysts for CO₂ Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study. *Inorg. Chem.*, **2015**, *54*, 7192-7198.
20. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B*, **2009**, *113*, 6378-6396.
21. Neese, F. Software update: the ORCA program system, version 4.0. *WIREs Comput Mol Sci*, **2018**, *8*:e1327.

18. Energies and cartesian coordinates of computed structures

Compound	$E_{el/DMSO}^{\omega B97M-V}$	$cor_{freq/gas}^{M06-L}$
H2	-1,16060318	-0,002379
N-Ethylpropionamide	-327,1461997	0,110841
1-(ethylamino)propan-1-ol <i>(Hemiaminal)</i>	-328,3087472	0,132223
Propionaldehyde	-193,1420016	0,048439
Ethylamine	-135,1541287	0,059867
1-Propanol	-194,3395313	0,072016
DMSO	-553,2044242	0,041764
DMSOK	-1152,525298	0,02382
C	-1405,368927	0,449007
D (P-arm)	-1404,168415	0,42697
D' (N-arm)	-1404,15928	0,42721
D'' (N-H)	-1404,168615	0,426626
E	-1731,329485	0,568019
F	-1731,337796	0,575461
G	-1957,394272	0,495024
H	-2556,71782	0,478113
I	-1732,516765	0,596468
TS1A	-1405,317061	0,443479
TS1B	-1732,48069	0,582696
TS2A1	-1732,490082	0,588693
TS2A2	-1732,494059	0,588426
TS2B	-1732,473229	0,585971
TS3A	-1732,480352	0,589552
TS3B	-1732,47278	0,596216
TS3C	-1732,473299	0,593157
TS3D1	-655,437025	0,271982
TS3D2	-655,4495396	0,268826

TS4	-2557,860074	0,49122
TS5	-2885,035977	0,630434
TS6	-2885,021165	0,637439
TS7	-1732,468108	0,591185

H2

H 0.054068000 -0.004785000 0.000000000

H 0.795232000 -0.070375000 0.000000000

Symmetry A

Frequency 4343.6623

Red. masses 1.0078

Frc consts 11.2033

IR Inten 0.0000

N-Ethylpropionamide

O	-2.677999000	0.589014000	-0.931598000
N	-1.734983000	1.713057000	0.786466000
C	0.402910000	2.007804000	-0.429528000
C	-0.403471000	1.189268000	0.557767000
C	-2.779753000	1.399388000	-0.029192000
C	-4.066822000	2.143216000	0.267763000
C	-5.282888000	1.446483000	-0.298382000
H	0.105568000	1.123167000	1.520286000
H	-0.527909000	0.172256000	0.186753000
H	1.391684000	1.575655000	-0.577433000
H	-0.098124000	2.038573000	-1.395617000
H	0.535894000	3.033127000	-0.084280000
H	-1.857848000	2.443502000	1.465622000
H	-3.966364000	3.143091000	-0.165793000
H	-4.162846000	2.300924000	1.344925000
H	-5.430381000	0.472181000	0.164553000

H -6.184254000 2.035321000 -0.139783000
 H -5.163653000 1.276904000 -1.365931000
 Symmetry A
 Frequency 27.8714
 Red. masses 2.1835
 Frc consts 0.0010
 IR Inten 0.3541
 Symmetry A
 Frequency 52.0595
 Red. masses 3.1329
 Frc consts 0.0050
 IR Inten 4.6012

1-(ethylamino)propan-1-ol (Hemiaminal)

O	-2.572850000	1.536349000	-1.426261000
N	-1.720205000	2.078177000	0.630983000
C	-5.307637000	1.404459000	-0.347351000
C	-4.132376000	2.017969000	0.382167000
C	-2.800859000	1.407932000	-0.025130000
C	-0.434629000	1.387013000	0.616719000
C	0.414941000	1.741102000	-0.585091000
H	-2.813955000	0.321601000	0.210708000
H	-3.093128000	0.857341000	-1.866924000
H	-5.244834000	1.588797000	-1.420068000
H	-6.254168000	1.819508000	-0.006976000
H	-5.353437000	0.324241000	-0.196102000
H	-4.256406000	1.894266000	1.461968000
H	-4.079438000	3.091708000	0.190229000
H	-1.995450000	2.307230000	1.573432000
H	0.598082000	2.813959000	-0.621759000
H	-0.081161000	1.461055000	-1.510920000

H 1.377420000 1.231243000 -0.540354000
 H -0.578039000 0.295932000 0.663239000
 H 0.096305000 1.661750000 1.530160000
 Symmetry A
 Frequency 9.6456
 Red. masses 2.3413
 Frc consts 0.0001
 IR Inten 0.0063
 Symmetry A
 Frequency 91.4888
 Red. masses 2.3051
 Frc consts 0.0114
 IR Inten 0.1010

Propionaldehyde

O -1.031202000 -1.025912000 0.370173000
 C -0.991659000 0.154308000 0.149493000
 C -2.189430000 1.021358000 -0.086604000
 C -3.508145000 0.288689000 -0.026222000
 H -0.015512000 0.693171000 0.106430000
 H -2.037942000 1.518208000 -1.051278000
 H -2.139052000 1.839723000 0.640089000
 H -3.650740000 -0.180273000 0.945470000
 H -4.344032000 0.961826000 -0.203880000
 H -3.548472000 -0.505745000 -0.768975000

Symmetry A
 Frequency 141.9667
 Red. masses 1.3610
 Frc consts 0.0162
 IR Inten 1.5124
 Symmetry A

Frequency 229.9964
Red. masses 1.3054
Frc consts 0.0407
IR Inten 0.3740

Ethylamine

N	-2.303970000	0.775472000	-0.141146000
C	-1.173425000	1.666782000	0.095670000
C	0.126886000	0.905469000	-0.008760000
H	-1.280642000	2.075269000	1.103165000
H	-1.143827000	2.533821000	-0.580910000
H	-3.174258000	1.288034000	-0.085248000
H	-2.256746000	0.409426000	-1.084525000
H	0.981574000	1.546932000	0.199844000
H	0.143779000	0.070691000	0.690489000
H	0.262243000	0.496164000	-1.011262000

Symmetry A
Frequency 244.7264
Red. masses 1.0691
Frc consts 0.0377
IR Inten 17.7916
Symmetry A
Frequency 244.7264
Red. masses 1.0691
Frc consts 0.0377
IR Inten 17.7916

1-Propanol

O	-0.632254000	-0.103965000	0.459900000
C	-0.730980000	1.155301000	-0.181753000
C	-1.962686000	1.939621000	0.224509000

C	-3.257455000	1.240860000	-0.141041000
H	-0.707334000	1.037482000	-1.274496000
H	0.174054000	1.696098000	0.096451000
H	-1.366906000	-0.645859000	0.157304000
H	-1.919991000	2.921055000	-0.254403000
H	-1.927472000	2.120091000	1.301243000
H	-3.361704000	0.289476000	0.383335000
H	-4.128902000	1.837873000	0.120939000
H	-3.311456000	1.036124000	-1.211916000

Symmetry A

Frequency 137.9107

Red. masses 1.7520

Frc consts 0.0196

IR Inten 2.8757

Symmetry A

Frequency 240.8423

Red. masses 1.2446

Frc consts 0.0425

IR Inten 11.9196

DMSO

S	-0.610180000	1.598287000	-0.438598000
O	-0.577524000	2.604603000	0.643941000
C	0.687853000	0.393145000	-0.076472000
C	-1.988155000	0.484451000	-0.080413000
H	0.578160000	0.039928000	0.947363000
H	0.636992000	-0.436595000	-0.778634000
H	1.640447000	0.904400000	-0.185816000
H	-2.903520000	1.058990000	-0.193520000
H	-1.991185000	-0.347436000	-0.781878000
H	-1.906231000	0.125517000	0.944026000

Symmetry A

Frequency 187.5592

Red. masses 1.0291

Frc consts 0.0213

IR Inten 0.0006

Symmetry A

Frequency 187.5592

Red. masses 1.0291

Frc consts 0.0213

IR Inten 0.0006

DMSOK

K -3.655854000 0.505583000 1.308328000

S -0.922677000 1.472878000 0.016650000

O -1.334454000 1.347439000 1.490830000

C -1.984251000 0.537282000 -0.941502000

C 0.630683000 0.544326000 0.029804000

H -1.674179000 -0.505362000 -1.046377000

H -2.132358000 1.014692000 -1.906154000

H 1.320720000 1.003362000 0.734913000

H 1.059280000 0.542032000 -0.970009000

H 0.413833000 -0.476261000 0.345469000

Symmetry A

Frequency 76.1953

Red. masses 4.6831

Frc consts 0.0160

IR Inten 18.0322

Symmetry A

Frequency 202.6573

Red. masses 3.5243

Frc consts 0.0853

IR Inten 16.8381

C

Ru	-0.358277000	-1.142975000	-0.177007000
P	-0.453184000	1.046327000	0.193143000
N	-0.609700000	-3.399707000	0.202777000
O	1.045988000	-0.935652000	-2.815214000
C	-2.653698000	-1.430826000	4.108223000
N	-1.364226000	-1.224957000	1.692402000
C	-1.871518000	1.109292000	1.400910000
H	-1.887367000	2.003090000	2.028633000
C	-1.948699000	-0.134918000	2.222252000
C	-2.594635000	-0.214433000	3.446668000
H	-3.053772000	0.670000000	3.867406000
C	-2.055459000	-2.544048000	3.540357000
H	-2.081945000	-3.507744000	4.031673000
C	-1.401945000	-2.404392000	2.328208000
C	-0.604808000	-3.489067000	1.676856000
H	-0.919622000	-4.469634000	2.044605000
H	0.435395000	-3.337200000	1.981779000
C	0.984900000	1.804665000	1.175987000
C	2.290100000	1.507118000	0.439058000
H	2.390066000	0.437483000	0.256362000
H	3.133423000	1.831336000	1.052915000
H	2.363483000	2.024951000	-0.515358000
C	1.025712000	1.066555000	2.517058000
H	0.181300000	1.324462000	3.158111000
H	1.933163000	1.352636000	3.052573000
H	1.048261000	-0.014210000	2.372162000
C	0.874358000	3.297058000	1.465293000
H	0.960824000	3.910499000	0.570497000
H	1.688719000	3.591794000	2.131651000
H	-0.057735000	3.556363000	1.969858000

C	-1.010788000	2.268396000	-1.140460000
C	-2.005586000	1.551009000	-2.053138000
H	-1.553153000	0.704635000	-2.563160000
H	-2.365854000	2.260905000	-2.801737000
H	-2.868585000	1.168226000	-1.508760000
C	-1.709414000	3.510666000	-0.585057000
H	-2.622227000	3.259384000	-0.045312000
H	-2.004743000	4.150122000	-1.419859000
H	-1.084329000	4.109002000	0.070542000
C	0.191617000	2.680441000	-1.988410000
H	0.885599000	3.323431000	-1.449806000
H	-0.157657000	3.240561000	-2.858348000
H	0.742364000	1.815688000	-2.358714000
H	0.296046000	-3.723515000	-0.118499000
C	-1.652337000	-4.224427000	-0.500225000
C	-1.410911000	-5.711328000	-0.249253000
H	-0.416343000	-6.010817000	-0.583746000
H	-2.135339000	-6.306999000	-0.803259000
H	-1.512736000	-5.983382000	0.800969000
C	-1.511002000	-3.933797000	-1.985354000
H	-1.716613000	-2.883954000	-2.186818000
H	-2.203750000	-4.550534000	-2.556959000
H	-0.501039000	-4.155494000	-2.335525000
C	-3.028497000	-3.811621000	-0.008029000
H	-3.189499000	-4.087054000	1.035418000
H	-3.797427000	-4.309918000	-0.596677000
H	-3.155540000	-2.733743000	-0.116998000
C	0.504480000	-1.029255000	-1.788180000
H	-3.163634000	-1.509744000	5.059233000
H	1.123081000	-1.448802000	0.643507000
H	-2.763917000	1.151198000	0.767988000

H -1.899600000 -1.017155000 -0.871213000

Symmetry A

Frequency 45.5271

Red. masses 5.3537

Frc consts 0.0065

IR Inten 1.2978

Symmetry A

Frequency 48.8007

Red. masses 3.6098

Frc consts 0.0051

IR Inten 0.2379

D

Ru -0.072315000 -1.187787000 0.190897000

P -0.251188000 1.034653000 0.617974000

N -0.586576000 -3.420192000 0.281920000

O 1.847518000 -0.946858000 -2.100902000

C -3.116630000 -1.558788000 3.957167000

N -1.360548000 -1.316584000 1.855496000

C -1.385812000 1.057979000 1.958469000

H -1.722009000 1.976403000 2.422466000

C -1.837409000 -0.155786000 2.446327000

C -2.761526000 -0.316834000 3.523165000

H -3.167967000 0.570696000 3.989171000

C -2.568716000 -2.713515000 3.364129000

H -2.812449000 -3.705988000 3.714974000

C -1.684347000 -2.530104000 2.329478000

C -0.926560000 -3.663261000 1.704693000

H -1.458618000 -4.606879000 1.848901000

H 0.026097000 -3.757601000 2.231527000

C 1.254819000 2.051176000 1.096313000

C 2.408734000 1.779495000 0.134688000

H	2.697196000	0.729669000	0.156618000
H	3.277563000	2.371006000	0.432663000
H	2.177124000	2.036388000	-0.897045000
C	1.663473000	1.566511000	2.487639000
H	0.913517000	1.810970000	3.237926000
H	2.605282000	2.040055000	2.773477000
H	1.810856000	0.486039000	2.505350000
C	0.956689000	3.545331000	1.158359000
H	0.781093000	3.973595000	0.172098000
H	1.812354000	4.071111000	1.588656000
H	0.092118000	3.765558000	1.785882000
C	-1.175449000	1.822894000	-0.836234000
C	-2.158096000	0.722229000	-1.253973000
H	-1.631766000	-0.158819000	-1.641511000
H	-2.813809000	1.076364000	-2.053376000
H	-2.789094000	0.418968000	-0.415795000
C	-1.987642000	3.051073000	-0.437772000
H	-2.657385000	2.830558000	0.392662000
H	-2.601755000	3.370831000	-1.283448000
H	-1.363321000	3.896232000	-0.156790000
C	-0.264547000	2.155818000	-2.010195000
H	0.392251000	2.997655000	-1.792804000
H	-0.868477000	2.439012000	-2.875966000
H	0.355333000	1.309724000	-2.306232000
H	0.279255000	-3.910164000	0.085068000
C	-1.593502000	-3.917407000	-0.721732000
C	-1.743450000	-5.433623000	-0.631490000
H	-0.786272000	-5.933666000	-0.787106000
H	-2.427296000	-5.788073000	-1.401488000
H	-2.145867000	-5.758575000	0.326367000
C	-1.065805000	-3.551710000	-2.101251000

H	-1.035006000	-2.471629000	-2.241685000
H	-1.705083000	-3.977139000	-2.873780000
H	-0.054992000	-3.931987000	-2.257116000
C	-2.926731000	-3.231890000	-0.472886000
H	-3.354750000	-3.499304000	0.492947000
H	-3.639749000	-3.519443000	-1.244383000
H	-2.822082000	-2.145752000	-0.500123000
C	1.089865000	-1.041043000	-1.220928000
H	-3.820486000	-1.659813000	4.774510000
H	1.188498000	-1.332405000	1.102797000

Symmetry A

Frequency 23.4821

Red. masses 3.7795

Frc consts 0.0012

IR Inten 1.2690

Symmetry A

Frequency 44.4695

Red. masses 4.0246

Frc consts 0.0047

IR Inten 0.1941

D'

Ru	-0.278614000	-1.220158000	0.027690000
P	-0.482510000	0.995744000	0.386565000
N	-0.524790000	-3.437129000	0.314208000
O	1.345025000	-0.915641000	-2.478769000
C	-2.268688000	-1.555588000	4.428070000
N	-1.347620000	-1.318657000	1.835507000
C	-1.778270000	1.038952000	1.705476000
H	-1.708731000	1.924636000	2.339841000
C	-1.781817000	-0.227124000	2.506235000
C	-2.242139000	-0.288480000	3.795009000

H	-2.591195000	0.602033000	4.296729000
C	-1.863632000	-2.670206000	3.769941000
H	-1.885361000	-3.641325000	4.246390000
C	-1.381899000	-2.581446000	2.421800000
C	-0.943983000	-3.643100000	1.685320000
H	-0.936728000	-4.648731000	2.078772000
C	0.990141000	1.875436000	1.162327000
C	2.237091000	1.618858000	0.317480000
H	2.441929000	0.553318000	0.229239000
H	3.099323000	2.089018000	0.794723000
H	2.157714000	2.025724000	-0.689043000
C	1.196004000	1.239455000	2.540389000
H	0.390897000	1.480495000	3.234201000
H	2.124086000	1.619357000	2.971577000
H	1.273493000	0.153951000	2.482460000
C	0.790901000	3.375574000	1.348854000
H	0.761659000	3.914536000	0.403194000
H	1.628954000	3.779499000	1.921041000
H	-0.117606000	3.609105000	1.905286000
C	-1.252114000	2.038956000	-0.985129000
C	-2.261699000	1.117847000	-1.676380000
H	-1.767112000	0.268557000	-2.148339000
H	-2.791600000	1.673004000	-2.453271000
H	-3.011862000	0.728474000	-0.985006000
C	-1.993978000	3.281039000	-0.493873000
H	-2.799095000	3.037875000	0.198534000
H	-2.452474000	3.781893000	-1.349490000
H	-1.343032000	4.004312000	-0.011031000
C	-0.189927000	2.438993000	-2.005536000
H	0.500639000	3.183816000	-1.612520000
H	-0.673949000	2.879658000	-2.879693000

H	0.390029000	1.583056000	-2.350210000
H	0.371770000	-3.890150000	0.158733000
C	-1.480232000	-3.980988000	-0.739020000
C	-2.025354000	-5.345173000	-0.337370000
H	-1.217106000	-6.057044000	-0.163614000
H	-2.651648000	-5.743929000	-1.134856000
H	-2.624661000	-5.284962000	0.568730000
C	-0.720731000	-4.109808000	-2.048088000
H	-0.341382000	-3.151735000	-2.395367000
H	-1.370613000	-4.515594000	-2.822375000
H	0.124982000	-4.791973000	-1.943991000
C	-2.614271000	-2.972773000	-0.853267000
H	-3.062718000	-2.789564000	0.123739000
H	-3.395252000	-3.326903000	-1.526460000
H	-2.254811000	-2.018006000	-1.261985000
C	0.700500000	-1.062540000	-1.519004000
H	-2.623818000	-1.633866000	5.448508000
H	1.088978000	-1.150661000	0.771237000
H	-2.734423000	1.114965000	1.179173000

Symmetry A

Frequency 36.0150

Red. masses 4.1251

Frc consts 0.0032

IR Inten 0.4682

Symmetry A

Frequency 39.9389

Red. masses 3.6660

Frc consts 0.0034

IR Inten 1.3307

D"

Ru	-1.651214000	-0.636938000	-0.271139000
P	-0.815026000	1.360727000	0.338930000
N	-1.830979000	-2.654342000	0.036240000
O	-0.881067000	-0.131215000	-3.118469000
C	-2.666784000	-0.978852000	4.479967000
N	-2.128491000	-0.709900000	1.800941000
C	-1.730577000	1.664080000	1.927825000
H	-1.224585000	2.344939000	2.615767000
C	-2.083373000	0.377907000	2.598815000
C	-2.349866000	0.265938000	3.950491000
H	-2.306080000	1.144218000	4.580213000
C	-2.693262000	-2.082863000	3.651056000
H	-2.916089000	-3.069274000	4.035565000
C	-2.409397000	-1.919735000	2.301305000
C	-2.349552000	-3.040772000	1.328802000
H	-3.361772000	-3.477842000	1.265557000
H	-1.747260000	-3.832332000	1.799476000
C	1.006290000	1.275288000	0.872445000
C	1.825070000	0.718796000	-0.292949000
H	1.422226000	-0.237427000	-0.629232000
H	2.855129000	0.556130000	0.031477000
H	1.853646000	1.387182000	-1.150772000
C	1.075452000	0.254868000	2.012075000
H	0.588159000	0.609204000	2.921254000
H	2.121858000	0.066538000	2.259947000
H	0.625135000	-0.697840000	1.728052000
C	1.614860000	2.581459000	1.367290000
H	1.714938000	3.325717000	0.579569000
H	2.619312000	2.388646000	1.752009000
H	1.041602000	3.023479000	2.183606000
C	-1.119350000	2.979222000	-0.594592000

C	-2.511033000	2.887689000	-1.221978000
H	-2.571045000	2.092156000	-1.960937000
H	-2.738758000	3.834515000	-1.716672000
H	-3.291437000	2.707072000	-0.481742000
C	-1.089254000	4.220893000	0.297550000
H	-1.873941000	4.202489000	1.053393000
H	-1.268423000	5.103929000	-0.319886000
H	-0.139457000	4.370871000	0.802637000
C	-0.102933000	3.127924000	-1.725321000
H	0.900890000	3.337916000	-1.360214000
H	-0.394634000	3.966605000	-2.361014000
H	-0.061782000	2.240660000	-2.356457000
C	-1.840762000	-3.788912000	-0.916437000
C	-1.181399000	-5.033214000	-0.305752000
H	-0.192025000	-4.792774000	0.085841000
H	-1.062605000	-5.804860000	-1.065605000
H	-1.770488000	-5.471653000	0.499043000
C	-1.058038000	-3.420742000	-2.167204000
H	-1.582508000	-2.678143000	-2.762579000
H	-0.917526000	-4.301620000	-2.793967000
H	-0.076955000	-3.019656000	-1.910604000
C	-3.275735000	-4.128563000	-1.333631000
H	-3.880279000	-4.468241000	-0.491965000
H	-3.286306000	-4.925553000	-2.078517000
H	-3.756402000	-3.250772000	-1.764835000
C	-1.181414000	-0.398808000	-2.024677000
H	-2.878315000	-1.082344000	5.536202000
H	-2.908045000	0.282656000	-0.568753000
H	-2.654889000	2.164111000	1.621555000

Symmetry A

Frequency 14.4189

Red. masses 2.9814

Frc consts 0.0004

IR Inten 0.1289

Symmetry A

Frequency 28.9312

Red. masses 3.9050

Frc consts 0.0019

IR Inten 0.3124

E

Ru	0.388636000	-1.271677000	-0.476773000
P	-0.470039000	0.786251000	-0.110793000
N	-1.141525000	-5.122178000	2.231788000
O	-1.083187000	-1.678602000	-3.017076000
C	-4.041605000	-2.083668000	2.175341000
N	-1.660289000	-1.783655000	0.775177000
C	-2.279595000	0.479342000	0.062723000
H	-2.831421000	1.304573000	0.518381000
C	-2.576451000	-0.798451000	0.786610000
C	-3.780463000	-0.926048000	1.470917000
H	-4.491208000	-0.110624000	1.449807000
C	-3.090678000	-3.086184000	2.184374000
H	-3.218597000	-4.000497000	2.745540000
C	-1.915536000	-2.906568000	1.470546000
C	-0.836300000	-3.941952000	1.448355000
H	0.060459000	-3.462821000	1.847499000
H	-0.586476000	-4.143758000	0.397243000
C	0.071870000	1.494215000	1.558690000
C	1.601003000	1.557066000	1.603699000
H	2.045240000	0.590780000	1.367980000
H	1.911102000	1.827523000	2.615667000

H	2.013156000	2.303657000	0.930096000
C	-0.381062000	0.506087000	2.639083000
H	-1.466230000	0.463163000	2.736461000
H	0.013824000	0.841527000	3.600328000
H	-0.001253000	-0.498792000	2.459712000
C	-0.513811000	2.861761000	1.893169000
H	-0.132602000	3.653094000	1.250361000
H	-0.239201000	3.123833000	2.917615000
H	-1.603719000	2.874011000	1.842532000
C	-0.431409000	2.152160000	-1.420465000
C	-0.580996000	1.492926000	-2.790276000
H	0.247997000	0.822644000	-3.006758000
H	-0.598514000	2.271889000	-3.555483000
H	-1.505142000	0.923755000	-2.886761000
C	-1.564488000	3.168068000	-1.268199000
H	-2.542731000	2.709966000	-1.411187000
H	-1.458963000	3.932609000	-2.040937000
H	-1.568427000	3.678165000	-0.309137000
C	0.918112000	2.865056000	-1.396412000
H	1.040867000	3.503933000	-0.523915000
H	1.000610000	3.504237000	-2.277817000
H	1.746422000	2.156371000	-1.424741000
H	-1.726913000	-5.744937000	1.686931000
C	0.021105000	-5.891360000	2.720285000
C	1.023735000	-6.202092000	1.608525000
H	0.550443000	-6.757891000	0.796601000
H	1.856364000	-6.799973000	1.981677000
H	1.436415000	-5.285952000	1.186000000
C	-0.534003000	-7.186896000	3.292584000
H	-1.261880000	-6.981419000	4.076765000
H	0.261463000	-7.799562000	3.714778000

H	-1.028180000	-7.777135000	2.518383000
C	0.701574000	-5.095809000	3.828216000
H	1.084195000	-4.139417000	3.470741000
H	1.547919000	-5.651470000	4.232168000
H	0.003279000	-4.893724000	4.639303000
C	-0.510185000	-1.457376000	-2.025531000
H	-4.970136000	-2.198089000	2.720503000
H	1.662426000	-0.720839000	-1.258474000
H	-2.642882000	0.400529000	-0.967629000
O	1.710362000	-1.649613000	1.281611000
C	2.220757000	-2.683662000	0.705652000
C	3.471120000	-3.268991000	1.294346000
H	3.749029000	-4.192148000	0.785194000
H	3.257985000	-3.534851000	2.332995000
C	4.612559000	-2.264006000	1.248796000
H	4.334659000	-1.350445000	1.771415000
H	5.512660000	-2.663938000	1.712464000
H	4.857132000	-1.993263000	0.221584000
N	1.592522000	-3.079843000	-0.367086000
C	2.029514000	-4.086101000	-1.296967000
H	2.700382000	-4.805446000	-0.813835000
H	1.150906000	-4.660180000	-1.612038000
C	2.705176000	-3.486487000	-2.514376000
H	3.606425000	-2.943761000	-2.227652000
H	2.983562000	-4.258406000	-3.231238000
H	2.042668000	-2.778713000	-3.011064000

Symmetry A

Frequency 16.4406

Red. masses 3.9331

Frc consts 0.0006

IR Inten 0.0170

Symmetry A
 Frequency 31.4756
 Red. masses 2.5407
 Frc consts 0.0015
 IR Inten 0.0499

F

Ru	-0.151233000	-0.911137000	-0.140915000
P	-0.444543000	1.312240000	0.008478000
N	-0.298468000	-3.175947000	0.336008000
O	1.206106000	-0.637309000	-2.787564000
C	-2.711483000	-1.021119000	3.997006000
N	-1.440856000	-0.958755000	1.564548000
C	-1.859526000	1.388797000	1.206534000
H	-1.893182000	2.315899000	1.780509000
C	-1.932605000	0.183533000	2.084581000
C	-2.553781000	0.180015000	3.322468000
H	-2.918140000	1.107830000	3.741736000
C	-2.293090000	-2.195397000	3.399759000
H	-2.438145000	-3.152887000	3.881387000
C	-1.664765000	-2.133654000	2.164466000
C	-1.296691000	-3.368463000	1.402915000
H	-2.222081000	-3.728533000	0.943510000
H	-0.986316000	-4.149741000	2.102717000
C	0.894924000	2.342864000	0.865540000
C	2.235934000	2.016059000	0.209513000
H	3.023417000	2.607207000	0.682178000
H	2.256669000	2.234938000	-0.857301000
H	2.469718000	0.962133000	0.356468000
C	0.954719000	1.859068000	2.314871000
H	0.077763000	2.154071000	2.892815000

H	1.824518000	2.305168000	2.801540000
H	1.075750000	0.780820000	2.359858000
C	0.664584000	3.849801000	0.888893000
H	0.716662000	4.311751000	-0.094587000
H	1.447669000	4.308369000	1.497114000
H	-0.288532000	4.119500000	1.346073000
C	-1.113938000	2.281251000	-1.476226000
C	-2.040510000	1.363072000	-2.273789000
H	-1.507033000	0.522586000	-2.709306000
H	-2.491336000	1.941029000	-3.083506000
H	-2.850169000	0.956498000	-1.666768000
C	-1.927596000	3.516582000	-1.083353000
H	-2.810331000	3.260174000	-0.498093000
H	-2.286508000	3.999976000	-1.994243000
H	-1.360754000	4.258129000	-0.530714000
C	0.042293000	2.689345000	-2.388776000
H	0.688938000	3.440900000	-1.940689000
H	-0.363208000	3.119540000	-3.306829000
H	0.656405000	1.836701000	-2.675202000
H	0.624676000	-3.321436000	0.761682000
C	-0.394226000	-4.234314000	-0.741952000
C	-0.437435000	-5.623495000	-0.105154000
H	0.411313000	-5.767978000	0.565333000
H	-0.381144000	-6.386770000	-0.879737000
H	-1.355781000	-5.802031000	0.453732000
C	0.861271000	-4.134336000	-1.593107000
H	0.916170000	-3.182039000	-2.114595000
H	0.854024000	-4.922095000	-2.345478000
H	1.758089000	-4.248347000	-0.983423000
C	-1.623587000	-3.990766000	-1.598945000
H	-2.553522000	-4.056759000	-1.032661000

H	-1.674873000	-4.741682000	-2.386609000
H	-1.579188000	-3.005338000	-2.059964000
C	0.733291000	-0.769597000	-1.732373000
H	-3.180808000	-1.040985000	4.971778000
H	-1.507234000	-0.966454000	-0.986545000
H	-2.761325000	1.378371000	0.585639000
O	2.625004000	-3.329987000	1.063636000
C	2.504544000	-2.136802000	0.712088000
C	3.365019000	-1.647228000	-0.433186000
H	3.069620000	-0.648382000	-0.747712000
H	3.240826000	-2.311418000	-1.291605000
C	4.820522000	-1.644307000	0.008843000
H	5.481829000	-1.323227000	-0.794914000
H	4.966790000	-0.965960000	0.851696000
H	5.127372000	-2.639251000	0.327963000
N	1.716116000	-1.230244000	1.331264000
C	1.357624000	-1.658764000	2.681684000
H	0.585049000	-0.990873000	3.071202000
H	0.935098000	-2.675459000	2.719999000
C	2.555421000	-1.608933000	3.613196000
H	2.975542000	-0.602331000	3.634212000
H	3.331729000	-2.293187000	3.275106000
H	2.281568000	-1.884288000	4.632326000

Symmetry A

Frequency 33.4966

Red. masses 3.5137

Frc consts 0.0023

IR Inten 0.2428

Symmetry A

Frequency 41.4174

Red. masses 3.3330

Frc consts 0.0034

IR Inten 0.2265

G

Ru	0.249778000	-0.675130000	-0.358880000
H	-0.176943000	-0.140337000	-1.764599000
P	-1.757925000	0.250522000	0.220010000
N	2.499496000	-0.741015000	-0.924733000
O	-0.888914000	-3.336969000	-1.129404000
C	1.857844000	3.861491000	0.375447000
N	0.937935000	1.285566000	0.078892000
C	-1.332143000	1.950757000	0.314948000
H	-2.066049000	2.719456000	0.519000000
C	0.009591000	2.292355000	0.281583000
C	0.518419000	3.616024000	0.442760000
H	-0.185372000	4.420387000	0.610195000
C	2.768877000	2.811732000	0.156534000
H	3.834733000	2.981367000	0.100554000
C	2.251191000	1.544350000	0.024085000
C	3.122170000	0.332495000	-0.110199000
H	3.272282000	-0.088183000	0.885479000
H	4.107406000	0.614500000	-0.488894000
C	-3.213154000	0.145347000	-0.991634000
C	-4.000145000	-1.152388000	-0.840346000
H	-3.353474000	-2.030116000	-0.850853000
H	-4.697171000	-1.251495000	-1.675876000
H	-4.594459000	-1.173824000	0.071900000
C	-2.654459000	0.204298000	-2.412993000
H	-1.989390000	1.058078000	-2.546609000
H	-3.484193000	0.308608000	-3.116495000
H	-2.103885000	-0.697902000	-2.672729000

C	-4.151812000	1.342980000	-0.831453000
H	-4.581939000	1.429138000	0.162980000
H	-4.980399000	1.241215000	-1.536269000
H	-3.639482000	2.276103000	-1.060268000
C	-2.382147000	-0.253532000	1.950651000
C	-1.256322000	0.165570000	2.899344000
H	-0.295440000	-0.255572000	2.602534000
H	-1.486731000	-0.178443000	3.911279000
H	-1.140248000	1.248170000	2.926385000
C	-3.654434000	0.465432000	2.382944000
H	-3.568130000	1.546748000	2.267665000
H	-3.844589000	0.267247000	3.441407000
H	-4.532716000	0.128752000	1.833863000
C	-2.576724000	-1.763172000	2.067028000
H	-3.464060000	-2.118055000	1.549568000
H	-2.687356000	-2.039117000	3.119535000
H	-1.722820000	-2.310378000	1.669579000
H	2.803312000	-1.624389000	-0.526153000
C	2.903314000	-0.761281000	-2.372408000
C	2.580223000	0.583562000	-3.001000000
H	1.531105000	0.835391000	-2.848203000
H	2.774740000	0.545829000	-4.072123000
H	3.186332000	1.387575000	-2.583111000
C	2.109039000	-1.867943000	-3.048277000
H	2.245352000	-2.823107000	-2.535575000
H	2.442489000	-1.996049000	-4.077658000
H	1.045763000	-1.638551000	-3.049162000
C	4.393846000	-1.071366000	-2.500957000
H	5.021440000	-0.313908000	-2.033729000
H	4.679358000	-1.120196000	-3.550987000
H	4.633619000	-2.036993000	-2.051108000

C	-0.437339000	-2.301303000	-0.820188000
H	2.224153000	4.874808000	0.489998000
C	1.898790000	-3.137705000	3.618919000
S	0.990930000	-2.827890000	2.100595000
O	1.476957000	-1.483264000	1.638906000
C	1.834125000	-4.045335000	1.079760000
H	1.541999000	-2.420480000	4.353372000
H	1.695965000	-4.148319000	3.966344000
H	2.963491000	-2.993178000	3.446615000
H	1.629159000	-5.043834000	1.459921000
H	1.429111000	-3.954268000	0.074440000
H	2.904928000	-3.845317000	1.085820000

Symmetry A

Frequency 26.2594

Red. masses 4.1534

Frc consts 0.0017

IR Inten 0.3316

Symmetry A

Frequency 37.0777

Red. masses 3.5659

Frc consts 0.0029

IR Inten 1.0407

H

Ru	0.015645000	-0.793997000	-0.512251000
H	-0.355239000	-0.042671000	-1.832270000
P	-1.913061000	0.265596000	0.141079000
N	2.220354000	-0.992611000	-1.126519000
O	-1.361453000	-3.283632000	-1.430338000
C	2.023433000	3.484135000	0.673134000
N	0.875694000	1.040123000	0.138740000

C	-1.322508000	1.876400000	0.486067000
H	-1.982199000	2.684616000	0.772512000
C	0.046111000	2.095383000	0.469953000
C	0.670243000	3.342984000	0.764960000
H	0.042618000	4.177745000	1.046800000
C	2.831544000	2.396316000	0.298095000
H	3.905433000	2.483272000	0.213998000
C	2.203970000	1.197852000	0.052172000
C	2.958891000	-0.059211000	-0.243482000
H	3.107854000	-0.581855000	0.701822000
H	3.951462000	0.175642000	-0.633909000
C	-3.320980000	0.480450000	-1.116102000
C	-4.266032000	-0.716010000	-1.135910000
H	-3.733666000	-1.661529000	-1.247643000
H	-4.946941000	-0.626177000	-1.985504000
H	-4.883395000	-0.771091000	-0.240838000
C	-2.713440000	0.635278000	-2.509121000
H	-1.950685000	1.414217000	-2.529120000
H	-3.501934000	0.917452000	-3.211218000
H	-2.261615000	-0.289512000	-2.863551000
C	-4.113697000	1.758111000	-0.831550000
H	-4.552472000	1.786589000	0.162649000
H	-4.932124000	1.836622000	-1.551000000
H	-3.487560000	2.641021000	-0.947800000
C	-2.691038000	-0.388210000	1.760073000
C	-1.530615000	-0.365004000	2.753581000
H	-0.712176000	-1.001762000	2.417979000
H	-1.863911000	-0.731853000	3.727292000
H	-1.129782000	0.639962000	2.880548000
C	-3.807504000	0.492545000	2.307730000
H	-3.501711000	1.537836000	2.364516000

H	-4.065891000	0.174908000	3.321482000
H	-4.717749000	0.430145000	1.712637000
C	-3.189534000	-1.832919000	1.621126000
H	-4.253863000	-1.890235000	1.405252000
H	-3.028636000	-2.382140000	2.554141000
H	-2.687524000	-2.360352000	0.807896000
H	2.386785000	-1.930768000	-0.768647000
C	2.625225000	-0.953417000	-2.569815000
C	2.457065000	0.462880000	-3.095048000
H	1.439057000	0.813988000	-2.926486000
H	2.658116000	0.488096000	-4.165349000
H	3.140347000	1.163265000	-2.614274000
C	1.716867000	-1.907793000	-3.329361000
H	1.734572000	-2.906201000	-2.887963000
H	2.047048000	-1.996126000	-4.364027000
H	0.687407000	-1.556043000	-3.319929000
C	4.072264000	-1.419365000	-2.726508000
H	4.779084000	-0.773795000	-2.207373000
H	4.355506000	-1.422761000	-3.778361000
H	4.198945000	-2.435130000	-2.347916000
C	-0.809624000	-2.290506000	-1.108970000
H	2.479085000	4.443726000	0.886492000
S	1.684071000	-2.040555000	2.629316000
O	1.230386000	-2.223379000	1.137660000
C	3.351684000	-2.715358000	2.504933000
H	3.271217000	-3.768858000	2.237000000
H	3.921644000	-2.191679000	1.739932000
H	3.845095000	-2.616239000	3.468336000
C	0.905002000	-3.167861000	3.607795000
H	0.466725000	-2.704784000	4.483593000
H	1.459138000	-4.082234000	3.805544000

K -0.681058000 -3.931374000 1.326868000

Symmetry A

Frequency 23.7864

Red. masses 4.5735

Frc consts 0.0015

IR Inten 0.3274

Symmetry A

Frequency 32.5873

Red. masses 4.6599

Frc consts 0.0029

IR Inten 1.6360

I

Ru -0.247426000 0.160921000 0.572136000

P 1.890704000 -0.252441000 0.075503000

N -2.507587000 -0.037741000 0.558715000

O 0.356805000 2.022359000 2.834777000

C -1.154895000 -3.153117000 -2.881658000

N -0.596290000 -1.300484000 -0.941841000

C 1.728203000 -1.906691000 -0.761941000

H 2.541970000 -2.127422000 -1.455953000

C 0.393709000 -2.078755000 -1.410122000

C 0.138272000 -3.011199000 -2.404413000

H 0.943581000 -3.624463000 -2.785224000

C -2.167199000 -2.366064000 -2.359948000

H -3.188167000 -2.463392000 -2.704231000

C -1.853725000 -1.432117000 -1.385140000

C -2.828553000 -0.451440000 -0.819153000

H -3.851235000 -0.822319000 -0.924916000

H -2.729204000 0.451018000 -1.428125000

C 2.656870000 0.840459000 -1.257525000

C	2.536984000	2.289474000	-0.788329000
H	1.503879000	2.514507000	-0.523715000
H	2.830237000	2.960237000	-1.598849000
H	3.172817000	2.511181000	0.066423000
C	1.762219000	0.667666000	-2.489529000
H	1.841610000	-0.331022000	-2.922839000
H	2.086209000	1.372378000	-3.259112000
H	0.718020000	0.886587000	-2.254819000
C	4.094793000	0.527069000	-1.650292000
H	4.808161000	0.739766000	-0.855694000
H	4.373274000	1.151010000	-2.503025000
H	4.226939000	-0.510840000	-1.960471000
C	3.171307000	-0.618596000	1.418034000
C	2.460928000	-1.306631000	2.583830000
H	1.721484000	-0.659625000	3.048973000
H	3.204871000	-1.578638000	3.336204000
H	1.947363000	-2.218813000	2.278990000
C	4.293727000	-1.545992000	0.947842000
H	3.922792000	-2.531992000	0.669201000
H	4.994256000	-1.695699000	1.772219000
H	4.862750000	-1.151774000	0.111291000
C	3.766746000	0.689857000	1.935118000
H	4.420886000	1.167377000	1.207713000
H	4.368532000	0.483360000	2.822595000
H	2.995185000	1.403347000	2.223947000
H	-2.681294000	0.978374000	0.624856000
C	-3.258776000	-0.741392000	1.641860000
C	-4.750873000	-0.424568000	1.543678000
H	-4.925430000	0.647204000	1.647900000
H	-5.298107000	-0.928315000	2.339952000
H	-5.188551000	-0.748552000	0.599679000

C	-2.735630000	-0.216818000	2.970801000
H	-1.695684000	-0.501313000	3.117131000
H	-3.328729000	-0.616814000	3.792993000
H	-2.795591000	0.872068000	3.010285000
C	-3.019644000	-2.238654000	1.534493000
H	-3.445164000	-2.656343000	0.620298000
H	-3.483374000	-2.755889000	2.373723000
H	-1.950035000	-2.450874000	1.548138000
C	0.108997000	1.316990000	1.942422000
H	-1.372692000	-3.882559000	-3.650959000
H	-0.077096000	-1.077972000	1.588884000
H	1.802799000	-2.641550000	0.045780000
O	-0.868417000	1.702866000	-0.956342000
C	-1.277905000	2.920291000	-0.525057000
H	-0.619205000	3.337273000	0.268034000
C	-1.302857000	3.941772000	-1.670448000
H	-1.682443000	4.893185000	-1.284790000
H	-2.015518000	3.604040000	-2.428313000
C	0.046195000	4.156564000	-2.318174000
H	-0.012298000	4.864100000	-3.145512000
H	0.771064000	4.549607000	-1.603634000
H	0.440197000	3.217138000	-2.703128000
N	-2.614493000	2.845719000	0.178233000
H	-2.685300000	3.602409000	0.848288000
C	-3.814011000	2.810629000	-0.658188000
H	-4.521166000	2.076059000	-0.247917000
H	-3.527451000	2.414526000	-1.635634000
C	-4.534839000	4.133975000	-0.818811000
H	-4.810748000	4.542988000	0.154770000
H	-3.914847000	4.872866000	-1.323419000
H	-5.454415000	4.019328000	-1.393514000

Symmetry A
 Frequency 33.2453
 Red. masses 3.5747
 Frc consts 0.0023
 IR Inten 0.089
 Symmetry A
 Frequency 41.8158
 Red. masses 3.8973
 Frc consts 0.0040
 IR Inten 0.1094

TS1A

Ru	-0.374998000	-1.148252000	-0.209325000
P	-0.501841000	1.050375000	0.195276000
N	-0.618674000	-3.382315000	0.134979000
O	1.153977000	-0.927902000	-2.782254000
C	-2.477715000	-1.454731000	4.135151000
N	-1.416732000	-1.233205000	1.621291000
C	-1.951176000	1.088967000	1.363265000
H	-1.987219000	1.983697000	1.988114000
C	-1.994845000	-0.158025000	2.188468000
C	-2.542297000	-0.236503000	3.451768000
H	-3.000944000	0.633399000	3.900542000
C	-1.869598000	-2.543534000	3.558996000
H	-1.806217000	-3.490511000	4.077993000
C	-1.323001000	-2.424023000	2.270939000
C	-0.507482000	-3.390599000	1.603375000
H	-0.448477000	-4.373121000	2.068224000
H	0.638155000	-2.522635000	1.444352000
C	0.925728000	1.775193000	1.213121000
C	2.237225000	1.441872000	0.501624000

H	2.335592000	0.365764000	0.357102000
H	3.076851000	1.780840000	1.112183000
H	2.325753000	1.919941000	-0.472174000
C	0.926261000	1.049261000	2.561275000
H	0.072040000	1.323129000	3.180688000
H	1.826788000	1.328533000	3.111587000
H	0.935746000	-0.033961000	2.439919000
C	0.842463000	3.271527000	1.491555000
H	0.952932000	3.878839000	0.595498000
H	1.653208000	3.552435000	2.167921000
H	-0.090976000	3.550521000	1.982207000
C	-1.015887000	2.281310000	-1.143389000
C	-1.994184000	1.574917000	-2.082950000
H	-1.526813000	0.743429000	-2.604323000
H	-2.347689000	2.294319000	-2.825027000
H	-2.866503000	1.182715000	-1.559668000
C	-1.720545000	3.521281000	-0.590714000
H	-2.643549000	3.267855000	-0.069878000
H	-1.997003000	4.170020000	-1.424604000
H	-1.104849000	4.109788000	0.082458000
C	0.205402000	2.691567000	-1.964442000
H	0.897086000	3.319677000	-1.406102000
H	-0.122451000	3.266795000	-2.832744000
H	0.752879000	1.825599000	-2.336701000
H	0.270196000	-3.708798000	-0.235768000
C	-1.687746000	-4.216420000	-0.508003000
C	-1.503798000	-5.684214000	-0.135092000
H	-0.514896000	-6.044680000	-0.423157000
H	-2.241600000	-6.300257000	-0.647994000
H	-1.627585000	-5.848611000	0.934551000
C	-1.524266000	-4.038600000	-2.009751000

H	-1.686281000	-2.999268000	-2.291774000
H	-2.235204000	-4.664561000	-2.547942000
H	-0.521179000	-4.322751000	-2.334277000
C	-3.053746000	-3.723430000	-0.063855000
H	-3.218205000	-3.892170000	0.999969000
H	-3.833314000	-4.257095000	-0.606428000
H	-3.160120000	-2.658301000	-0.268022000
C	0.572809000	-1.031667000	-1.779591000
H	-2.909429000	-1.538081000	5.124551000
H	1.084707000	-1.786607000	0.937954000
H	-2.832710000	1.120039000	0.715177000
H	-1.735290000	-0.932643000	-1.039594000

Symmetry A

Frequency -1412.0756

Red. masses 1.1212

Frc consts 1.3172

IR Inten 1977.9050

Symmetry A

Frequency 45.6520

Red. masses 5.0670

Frc consts 0.0062

IR Inten 1.0343

TS1B

Ru	0.021943000	-0.964781000	-0.297406000
P	-0.391465000	1.193173000	0.242147000
N	0.248610000	-3.203974000	-0.017790000
O	1.099937000	-0.262037000	-2.999498000
C	-2.091735000	-1.837457000	4.014131000
N	-1.049140000	-1.328466000	1.525658000
C	-1.690554000	0.994965000	1.542466000
H	-1.722215000	1.827416000	2.247316000

C	-1.591095000	-0.322834000	2.238551000
C	-2.101478000	-0.547218000	3.503569000
H	-2.510841000	0.277140000	4.071250000
C	-1.612122000	-2.869968000	3.237491000
H	-1.604815000	-3.889154000	3.597478000
C	-1.089163000	-2.583288000	1.984111000
C	-0.662314000	-3.658671000	1.045013000
H	-1.570181000	-4.056851000	0.578801000
H	-0.217454000	-4.474623000	1.619894000
C	0.995196000	2.073525000	1.188157000
C	2.281754000	2.053530000	0.363044000
H	3.090407000	2.492002000	0.950924000
H	2.197304000	2.630680000	-0.555777000
H	2.581813000	1.043165000	0.094565000
C	1.212090000	1.281366000	2.484857000
H	0.403820000	1.445678000	3.198124000
H	2.130741000	1.629873000	2.960598000
H	1.309040000	0.205272000	2.336009000
C	0.677442000	3.514879000	1.575538000
H	0.631449000	4.183338000	0.717719000
H	1.471185000	3.886591000	2.227214000
H	-0.256240000	3.602862000	2.132102000
C	-1.204965000	2.374137000	-0.985313000
C	-2.146953000	1.543882000	-1.859105000
H	-1.609600000	0.813164000	-2.458175000
H	-2.683145000	2.214622000	-2.533688000
H	-2.889281000	1.001324000	-1.272782000
C	-2.034261000	3.475871000	-0.323574000
H	-2.854941000	3.074454000	0.270053000
H	-2.483916000	4.091685000	-1.105151000
H	-1.451973000	4.137792000	0.309864000

C	-0.140198000	2.996375000	-1.886419000
H	0.483598000	3.715372000	-1.358071000
H	-0.629001000	3.532898000	-2.701987000
H	0.507147000	2.243725000	-2.335815000
H	1.199321000	-3.196656000	0.412274000
C	0.332785000	-4.164636000	-1.173798000
C	0.480054000	-5.599016000	-0.663005000
H	1.307394000	-5.677169000	0.044132000
H	0.688330000	-6.268364000	-1.496571000
H	-0.423155000	-5.963704000	-0.175297000
C	1.581981000	-3.809104000	-1.966839000
H	1.515336000	-2.816284000	-2.402949000
H	1.718555000	-4.520194000	-2.780649000
H	2.467700000	-3.843230000	-1.332961000
C	-0.900210000	-4.032569000	-2.050852000
H	-1.818666000	-4.258220000	-1.507822000
H	-0.839280000	-4.727358000	-2.888335000
H	-0.984888000	-3.020428000	-2.444474000
C	0.724665000	-0.563532000	-1.941323000
H	-2.473462000	-2.032273000	5.007773000
H	-1.422625000	-1.050986000	-0.981196000
H	-2.644081000	1.010306000	1.004839000
O	1.389139000	-2.435466000	2.852411000
C	2.558918000	-2.714369000	2.501205000
C	3.637464000	-2.765307000	3.580495000
H	4.366723000	-1.975733000	3.371035000
H	4.203793000	-3.695959000	3.487684000
C	3.085711000	-2.609093000	4.978896000
H	3.879528000	-2.633115000	5.725627000
H	2.545516000	-1.669435000	5.080435000
H	2.375478000	-3.400958000	5.211689000

N	2.854128000	-2.914942000	1.220664000
C	4.207286000	-3.197450000	0.801965000
H	4.347563000	-2.767317000	-0.196959000
H	4.960842000	-2.707772000	1.432590000
C	4.505113000	-4.686705000	0.734477000
H	3.813888000	-5.189008000	0.056140000
H	4.392973000	-5.154089000	1.713537000
H	5.519038000	-4.883417000	0.383494000
H	1.716028000	-0.722133000	0.518415000
H	1.989060000	-1.489468000	0.604380000

Symmetry A

Frequency -34.7307

Red. masses 3.8387

Frc consts 0.0027

IR Inten 21.1634

Symmetry A

Frequency 17.5867

Red. masses 3.8380

Frc consts 0.0007

IR Inten 1.5828

TS2A1

Ru	-0.293887000	-0.851420000	0.061984000
P	-0.372466000	1.388122000	-0.105805000
N	-0.607719000	-2.939194000	0.844329000
O	1.540057000	-1.047415000	-2.294075000
C	-3.024169000	-0.166088000	4.017500000
N	-1.659168000	-0.529341000	1.664854000
C	-1.803504000	1.783519000	1.009302000
H	-1.737303000	2.771211000	1.468052000
C	-2.047022000	0.710041000	2.019270000

C	-2.718983000	0.920226000	3.212038000
H	-3.008210000	1.923245000	3.494879000
C	-2.688114000	-1.439943000	3.597083000
H	-2.938972000	-2.310659000	4.188133000
C	-2.009948000	-1.593532000	2.397140000
C	-1.730614000	-2.932490000	1.793625000
H	-2.640852000	-3.235346000	1.264525000
H	-1.578408000	-3.664753000	2.592534000
C	1.055997000	2.351646000	0.686156000
C	2.363523000	1.801837000	0.118155000
H	3.209785000	2.241343000	0.651394000
H	2.488843000	2.027287000	-0.939703000
H	2.413083000	0.719595000	0.234864000
C	0.986164000	2.021328000	2.178501000
H	0.192519000	2.574929000	2.682604000
H	1.926918000	2.301132000	2.659035000
H	0.819663000	0.958698000	2.353907000
C	1.023634000	3.868094000	0.541193000
H	1.171335000	4.204107000	-0.483157000
H	1.834503000	4.295695000	1.135980000
H	0.095084000	4.301457000	0.915281000
C	-0.869253000	2.238396000	-1.722605000
C	-1.876513000	1.338619000	-2.438637000
H	-1.434898000	0.389909000	-2.732041000
H	-2.229712000	1.851309000	-3.336185000
H	-2.747004000	1.111614000	-1.821873000
C	-1.529681000	3.603811000	-1.524088000
H	-2.452249000	3.536159000	-0.947980000
H	-1.800745000	4.007077000	-2.502130000
H	-0.886432000	4.334805000	-1.044875000
C	0.358027000	2.380554000	-2.621792000

H	1.069110000	3.115047000	-2.248060000
H	0.041006000	2.715488000	-3.611628000
H	0.880798000	1.433367000	-2.751373000
H	0.243436000	-3.005408000	1.444401000
C	-0.566868000	-4.172530000	-0.019509000
C	-0.792781000	-5.422196000	0.833595000
H	-0.099960000	-5.448993000	1.675981000
H	-0.622065000	-6.313976000	0.232344000
H	-1.809885000	-5.486612000	1.219626000
C	0.831698000	-4.246757000	-0.615558000
H	1.017110000	-3.433869000	-1.312089000
H	0.953043000	-5.182859000	-1.159389000
H	1.588084000	-4.203799000	0.169037000
C	-1.609593000	-4.079892000	-1.119033000
H	-2.622929000	-4.007789000	-0.721159000
H	-1.570631000	-4.970669000	-1.745943000
H	-1.431707000	-3.204421000	-1.741458000
C	0.842395000	-1.007262000	-1.361581000
H	-3.536912000	-0.019403000	4.959235000
H	-1.560829000	-0.967135000	-0.944960000
H	-2.681555000	1.808690000	0.355789000
O	1.463949000	-2.900401000	2.512680000
C	1.672614000	-1.651290000	2.596100000
H	1.003647000	-1.009177000	1.463077000
C	3.072402000	-1.131922000	2.269954000
H	3.701031000	-1.412751000	3.123364000
H	3.064342000	-0.038778000	2.239664000
N	1.077559000	-0.984773000	3.723350000
H	1.639933000	-0.209378000	4.046529000
C	0.637237000	-1.821079000	4.825103000
H	-0.157193000	-2.477611000	4.465375000

H	1.432269000	-2.496660000	5.169975000
C	3.628846000	-1.715469000	0.995884000
H	4.615985000	-1.317383000	0.765283000
H	3.704873000	-2.798665000	1.075711000
H	2.972686000	-1.498542000	0.151134000
C	0.140433000	-0.964765000	5.965079000
H	-0.219744000	-1.576761000	6.790873000
H	0.934148000	-0.326307000	6.357588000
H	-0.672184000	-0.313521000	5.641848000

Symmetry A

Frequency -708.5330

Red. masses 1.7539

Frc consts 0.5188

IR Inten 2092.9333

Symmetry A

Frequency 21.2294

Red. masses 3.1980

Frc consts 0.0008

IR Inten 0.0509

TS2A2

Ru	-0.224071000	-0.910218000	-0.007635000
P	-0.456159000	1.340766000	0.071917000
N	-0.289938000	-3.023047000	0.601978000
O	1.455821000	-0.720996000	-2.476686000
C	-3.038463000	-0.837605000	3.952882000
N	-1.597876000	-0.846131000	1.617460000
C	-1.918836000	1.510043000	1.200942000
H	-1.922931000	2.441343000	1.769432000
C	-2.098580000	0.317810000	2.082204000
C	-2.805350000	0.349071000	3.271167000

H	-3.178605000	1.291345000	3.648244000
C	-2.587834000	-2.028954000	3.419797000
H	-2.768887000	-2.972172000	3.917058000
C	-1.864126000	-2.005350000	2.235085000
C	-1.381729000	-3.240092000	1.556911000
H	-2.254037000	-3.667995000	1.046056000
H	-1.096182000	-3.973041000	2.320307000
C	0.911349000	2.282912000	0.979624000
C	2.249365000	1.895195000	0.349714000
H	3.065130000	2.342281000	0.921363000
H	2.345482000	2.230651000	-0.681591000
H	2.388431000	0.813734000	0.363115000
C	0.897855000	1.776002000	2.422221000
H	0.009539000	2.095627000	2.969724000
H	1.764861000	2.175102000	2.952012000
H	0.978416000	0.691860000	2.481678000
C	0.764378000	3.799197000	1.010629000
H	0.870765000	4.259878000	0.030686000
H	1.549630000	4.215530000	1.645596000
H	-0.188399000	4.115448000	1.437604000
C	-1.009129000	2.324825000	-1.446362000
C	-1.943915000	1.428923000	-2.260595000
H	-1.427279000	0.558777000	-2.658281000
H	-2.342284000	2.003477000	-3.099503000
H	-2.792214000	1.068238000	-1.677001000
C	-1.771848000	3.606911000	-1.108106000
H	-2.694219000	3.408634000	-0.562648000
H	-2.059287000	4.099295000	-2.039468000
H	-1.189336000	4.321671000	-0.535279000
C	0.202412000	2.657804000	-2.315622000
H	0.854677000	3.399363000	-1.858230000

H	-0.141687000	3.074610000	-3.264363000
H	0.796573000	1.774321000	-2.545935000
H	0.706847000	-3.089294000	1.264458000
C	-0.186803000	-4.166769000	-0.372630000
C	-0.294419000	-5.507988000	0.361006000
H	0.416194000	-5.556052000	1.186825000
H	-0.061537000	-6.319883000	-0.326607000
H	-1.293808000	-5.698459000	0.751268000
C	1.184371000	-4.115388000	-1.027515000
H	1.337457000	-3.194675000	-1.583847000
H	1.287761000	-4.943983000	-1.727766000
H	1.967963000	-4.194473000	-0.276387000
C	-1.272136000	-4.060920000	-1.434910000
H	-2.273498000	-4.039086000	-1.001726000
H	-1.229354000	-4.917950000	-2.107949000
H	-1.143019000	-3.153261000	-2.023209000
C	0.842613000	-0.836808000	-1.495022000
H	-3.582197000	-0.828515000	4.888525000
H	-1.456829000	-0.966862000	-0.984847000
H	-2.790724000	1.553394000	0.540511000
O	1.779038000	-3.091092000	2.010593000
C	2.159557000	-1.815988000	2.124990000
H	1.461135000	-1.137304000	1.479348000
C	3.580831000	-1.524724000	1.636214000
H	4.262442000	-2.018244000	2.337296000
H	3.769749000	-0.452595000	1.734076000
C	3.857937000	-2.003043000	0.233250000
H	4.863515000	-1.737982000	-0.091888000
H	3.757102000	-3.084588000	0.167592000
H	3.158140000	-1.566880000	-0.481908000
N	2.063864000	-1.225999000	3.475525000

H	2.810501000	-1.639029000	4.025773000
C	0.804450000	-1.457970000	4.147621000
H	0.037210000	-0.910070000	3.591603000
H	0.503019000	-2.517085000	4.124546000
C	0.841318000	-0.945614000	5.567817000
H	1.076983000	0.118998000	5.591229000
H	1.602527000	-1.462059000	6.154700000
H	-0.114182000	-1.094976000	6.070588000

Symmetry A

Frequency -1301.9828

Red. masses 1.1088

Frc consts 1.1075

IR Inten 1492.6138

Symmetry A

Frequency 26.9402

Red. masses 3.4272

Frc consts 0.0015

IR Inten 0.1468

TS2B

Ru	0.851983000	-1.196865000	0.094397000
P	-0.242036000	0.748651000	0.128421000
N	-0.635450000	-4.361049000	0.771146000
O	2.448592000	-0.350936000	-2.251112000
C	-1.807405000	-1.632786000	4.403444000
N	-0.663088000	-1.725190000	1.866455000
C	-1.646571000	0.421232000	1.265929000
H	-2.028549000	1.324954000	1.743645000
C	-1.368287000	-0.646165000	2.272501000
C	-1.922723000	-0.559660000	3.540278000
H	-2.452447000	0.338631000	3.827685000

C	-1.220419000	-2.787717000	3.932052000
H	-1.188427000	-3.684943000	4.535297000
C	-0.680175000	-2.823702000	2.650319000
C	-0.166840000	-4.127796000	2.118084000
H	-0.553035000	-4.913635000	2.772151000
H	0.928485000	-4.156191000	2.210688000
C	0.678124000	2.171745000	0.987988000
C	2.053244000	2.341330000	0.343401000
H	2.619808000	1.411575000	0.384539000
H	2.616445000	3.104355000	0.885067000
H	1.997070000	2.653395000	-0.697938000
C	0.876292000	1.758250000	2.449001000
H	-0.059069000	1.766422000	3.009662000
H	1.546774000	2.471388000	2.932602000
H	1.324709000	0.767355000	2.535536000
C	-0.056601000	3.508660000	0.986283000
H	-0.141112000	3.946125000	-0.006096000
H	0.500212000	4.219503000	1.601050000
H	-1.056714000	3.434808000	1.415200000
C	-1.120257000	1.413095000	-1.413477000
C	-1.642844000	0.209395000	-2.199090000
H	-0.835020000	-0.408905000	-2.581164000
H	-2.233741000	0.572527000	-3.042893000
H	-2.282231000	-0.437977000	-1.598182000
C	-2.318118000	2.311949000	-1.098701000
H	-3.094246000	1.785087000	-0.544551000
H	-2.769306000	2.632154000	-2.040189000
H	-2.060669000	3.210590000	-0.546889000
C	-0.131639000	2.164366000	-2.303592000
H	0.184423000	3.113811000	-1.874883000
H	-0.611073000	2.388393000	-3.258737000

H	0.757261000	1.572907000	-2.519726000
H	-0.252780000	-3.633672000	0.173163000
C	-0.301905000	-5.675966000	0.189690000
C	1.134685000	-6.123752000	0.469463000
H	1.847630000	-5.358067000	0.164914000
H	1.359330000	-7.044092000	-0.070894000
H	1.293559000	-6.329288000	1.529621000
C	-0.500141000	-5.524049000	-1.311685000
H	-1.505848000	-5.165643000	-1.530870000
H	-0.352465000	-6.473801000	-1.824846000
H	0.209692000	-4.803165000	-1.721108000
C	-1.279177000	-6.709337000	0.739958000
H	-1.190062000	-6.808623000	1.822688000
H	-1.088458000	-7.693083000	0.309777000
H	-2.305790000	-6.425025000	0.512601000
C	1.816762000	-0.683562000	-1.328437000
H	-2.216341000	-1.585340000	5.404530000
H	-0.266631000	-1.860833000	-0.913213000
H	-2.449352000	0.045030000	0.624202000
O	2.031034000	-2.984106000	0.561425000
C	2.834995000	-2.209153000	1.205526000
H	2.077528000	-0.732889000	1.283525000
C	2.912815000	-2.327936000	2.717599000
H	1.895944000	-2.293719000	3.108465000
H	3.432194000	-1.464996000	3.137590000
C	3.605802000	-3.620435000	3.115930000
H	4.642132000	-3.632018000	2.780323000
H	3.599837000	-3.753330000	4.196678000
H	3.109045000	-4.481454000	2.667689000
N	4.041789000	-1.907320000	0.586484000
H	3.949531000	-1.966941000	-0.418735000

C	4.818368000	-0.766049000	1.033374000
H	4.136811000	0.038181000	1.354124000
H	5.403530000	-1.043602000	1.915362000
C	5.725959000	-0.267161000	-0.063944000
H	5.146020000	0.066899000	-0.925195000
H	6.326630000	0.572613000	0.278890000
H	6.406031000	-1.049455000	-0.400028000

Symmetry A

Frequency -519.3920

Red. masses 1.7510

Frc consts 0.2783

IR Inten 503.5995

Symmetry A

Frequency 25.2140

Red. masses 3.9772

Frc consts 0.0015

IR Inten 0.0395

TS3A

Ru	0.204689000	-0.945296000	-0.063353000
P	-0.366492000	1.217784000	0.080044000
N	0.119839000	-3.202590000	0.307218000
O	2.235056000	-0.573414000	-2.232089000
C	-3.075745000	-1.454509000	3.495555000
N	-1.309272000	-1.152428000	1.421754000
C	-2.039944000	1.068396000	0.867477000
H	-2.355322000	1.974033000	1.389470000
C	-2.128546000	-0.139003000	1.748771000
C	-3.018354000	-0.243702000	2.799862000
H	-3.663969000	0.584676000	3.054173000
C	-2.272463000	-2.504348000	3.129169000

H	-2.336957000	-3.458455000	3.636952000
C	-1.357531000	-2.351727000	2.063721000
C	-0.425317000	-3.350657000	1.669126000
H	-0.729871000	-4.364809000	1.926440000
H	0.874806000	-3.138223000	2.542320000
C	0.598762000	2.276607000	1.317612000
C	2.085899000	2.153665000	0.986725000
H	2.670120000	2.685776000	1.741953000
H	2.340931000	2.579304000	0.017607000
H	2.383812000	1.105869000	1.000549000
C	0.362246000	1.641699000	2.692208000
H	-0.655721000	1.798926000	3.050866000
H	1.035236000	2.109865000	3.414798000
H	0.579872000	0.574120000	2.679128000
C	0.195433000	3.743981000	1.402527000
H	0.434278000	4.305823000	0.501277000
H	0.743473000	4.212271000	2.224002000
H	-0.866752000	3.872860000	1.615891000
C	-0.724384000	2.231830000	-1.475122000
C	-1.299955000	1.291874000	-2.534989000
H	-0.583889000	0.530914000	-2.834798000
H	-1.569955000	1.879761000	-3.415377000
H	-2.197292000	0.776799000	-2.191152000
C	-1.743333000	3.350324000	-1.250404000
H	-2.713130000	2.963289000	-0.938678000
H	-1.902226000	3.876581000	-2.194197000
H	-1.425764000	4.089019000	-0.521136000
C	0.578114000	2.813407000	-2.021746000
H	0.987179000	3.596986000	-1.386552000
H	0.390229000	3.257702000	-3.001540000
H	1.341233000	2.046421000	-2.153332000

H	1.111020000	-3.436075000	0.325128000
C	-0.472292000	-4.120899000	-0.738110000
C	-0.170205000	-5.574207000	-0.377746000
H	0.905974000	-5.744340000	-0.304625000
H	-0.555161000	-6.242611000	-1.147231000
H	-0.627297000	-5.870236000	0.565208000
C	0.191154000	-3.792863000	-2.066015000
H	-0.085701000	-2.796419000	-2.403131000
H	-0.104919000	-4.515891000	-2.826080000
H	1.279670000	-3.828088000	-1.982388000
C	-1.970404000	-3.893251000	-0.816363000
H	-2.467923000	-4.168561000	0.113353000
H	-2.396151000	-4.499736000	-1.615114000
H	-2.184170000	-2.845693000	-1.025067000
C	1.454981000	-0.728992000	-1.379560000
H	-3.776777000	-1.572253000	4.312883000
H	-0.946265000	-1.033802000	-1.164767000
H	-2.736335000	0.929974000	0.034341000
O	1.730037000	-0.977107000	1.629830000
C	2.562974000	-1.941090000	1.915511000
C	3.938014000	-1.470365000	2.384517000
H	4.490688000	-2.294018000	2.850213000
H	3.790369000	-0.703783000	3.149993000
C	4.725035000	-0.901202000	1.222174000
H	5.695548000	-0.520391000	1.535782000
H	4.898230000	-1.657667000	0.455300000
H	4.178804000	-0.085155000	0.751714000
N	1.910587000	-2.854626000	3.040156000
C	1.623415000	-2.148698000	4.297208000
H	2.559500000	-1.831399000	4.761441000
H	1.083470000	-1.245390000	4.009396000

C	0.810682000	-3.003109000	5.239761000
H	1.346510000	-3.908353000	5.528406000
H	-0.132968000	-3.300836000	4.783861000
H	0.579324000	-2.455025000	6.151023000
H	2.728940000	-2.704776000	1.112273000
H	2.467028000	-3.688103000	3.212537000

Symmetry A

Frequency -1118.7072

Red. masses 1.1885

Frc consts 0.8763

IR Inten 4009.4986

Symmetry A

Frequency 33.5841

Red. masses 3.5878

Frc consts 0.0024

IR Inten 0.3054

TS3B

Ru	0.366562000	-0.975903000	-0.016907000
P	-0.292730000	1.187710000	-0.048410000
N	0.195165000	-3.198728000	0.370690000
O	1.928077000	-0.903158000	-2.566592000
C	-2.968726000	-1.415929000	3.528924000
N	-1.078459000	-1.114838000	1.557462000
C	-1.926810000	1.015747000	0.826503000
H	-2.281411000	1.939485000	1.285941000
C	-1.960664000	-0.124718000	1.785247000
C	-2.901933000	-0.241618000	2.796701000
H	-3.589967000	0.571624000	2.983802000
C	-2.118986000	-2.461892000	3.212499000
H	-2.179919000	-3.411415000	3.727381000
C	-1.179112000	-2.281440000	2.210882000

C	-0.196664000	-3.323512000	1.787537000
H	-0.584967000	-4.316398000	2.028416000
H	0.703713000	-3.203182000	2.391184000
C	0.556154000	2.501416000	1.038411000
C	1.974384000	2.772612000	0.529155000
H	2.609128000	3.106608000	1.352309000
H	1.987437000	3.558767000	-0.221883000
H	2.438517000	1.893455000	0.090904000
C	0.609327000	1.844600000	2.423584000
H	-0.374099000	1.824632000	2.896497000
H	1.269080000	2.418090000	3.077377000
H	0.980194000	0.819613000	2.379803000
C	-0.159576000	3.841148000	1.182800000
H	-0.115108000	4.433436000	0.270540000
H	0.337956000	4.425526000	1.961027000
H	-1.204108000	3.744392000	1.480130000
C	-0.813061000	1.997732000	-1.681276000
C	-1.323354000	0.922087000	-2.639879000
H	-0.553767000	0.201975000	-2.904773000
H	-1.663748000	1.410008000	-3.556143000
H	-2.166188000	0.366507000	-2.228281000
C	-1.935326000	3.026029000	-1.521642000
H	-2.865703000	2.569675000	-1.185003000
H	-2.141069000	3.473142000	-2.496437000
H	-1.694131000	3.837147000	-0.842240000
C	0.406063000	2.665275000	-2.315580000
H	0.684297000	3.583208000	-1.801332000
H	0.175711000	2.931934000	-3.348660000
H	1.274302000	2.005084000	-2.335497000
H	1.197472000	-3.436845000	0.255055000
C	-0.554014000	-4.109526000	-0.561370000

C	-0.200458000	-5.562076000	-0.238393000
H	0.876435000	-5.716664000	-0.311070000
H	-0.687153000	-6.233121000	-0.945249000
H	-0.522769000	-5.863551000	0.758166000
C	-0.084322000	-3.802413000	-1.975337000
H	-0.422525000	-2.819171000	-2.295922000
H	-0.480468000	-4.545495000	-2.667109000
H	1.004162000	-3.826351000	-2.035311000
C	-2.050166000	-3.876455000	-0.433827000
H	-2.432858000	-4.170929000	0.545168000
H	-2.584141000	-4.466600000	-1.177733000
H	-2.288520000	-2.824848000	-0.598917000
C	1.380844000	-0.926696000	-1.543903000
H	-3.701747000	-1.525604000	4.317360000
H	-0.937305000	-1.060525000	-0.945752000
H	-2.639150000	0.776391000	0.029845000
O	2.937156000	-3.458459000	0.048998000
C	3.098748000	-3.106164000	1.238804000
C	4.488457000	-2.984616000	1.836596000
H	5.064706000	-2.202775000	1.342624000
H	4.988573000	-3.919137000	1.567731000
C	4.484664000	-2.820371000	3.341840000
H	5.492343000	-2.771082000	3.751915000
H	3.961717000	-1.914484000	3.651818000
H	3.978708000	-3.659431000	3.822779000
N	2.264078000	-1.287503000	1.437770000
C	3.332173000	-0.289298000	1.394914000
H	2.966564000	0.700248000	1.689762000
H	4.104189000	-0.516351000	2.141520000
C	3.996249000	-0.201265000	0.037030000
H	3.377961000	0.321016000	-0.691531000

H	4.188587000	-1.192362000	-0.373212000
H	4.942769000	0.336286000	0.105326000
H	2.419555000	-3.523448000	2.021832000
H	1.920890000	-1.285760000	2.401278000

Symmetry A

Frequency -226.8343

Red. masses 6.6417

Frc consts 0.2013

IR Inten 127.7002

Symmetry A

Frequency 32.8761

Red. masses 3.9502

Frc consts 0.0025

IR Inten 0.1194

TS3C

Ru	0.113105000	-0.984615000	-0.147611000
P	-0.333630000	1.211479000	0.018612000
N	-0.063990000	-3.233208000	0.234138000
O	1.770515000	-0.675289000	-2.615598000
C	-3.178731000	-1.365093000	3.452227000
N	-1.327265000	-1.112315000	1.439789000
C	-1.951450000	1.160663000	0.919875000
H	-2.163044000	2.073554000	1.479848000
C	-2.091369000	-0.057298000	1.773220000
C	-3.009877000	-0.151825000	2.805692000
H	-3.597118000	0.713760000	3.080553000
C	-2.439620000	-2.459402000	3.043676000
H	-2.557436000	-3.425875000	3.514455000
C	-1.506286000	-2.296865000	2.034148000
C	-0.570037000	-3.377396000	1.619317000

H	-1.018947000	-4.357636000	1.789829000
H	0.272441000	-3.280516000	2.303588000
C	0.750628000	2.247897000	1.176139000
C	2.206287000	2.157863000	0.707689000
H	2.876138000	2.423015000	1.528053000
H	2.411353000	2.844183000	-0.111589000
H	2.476067000	1.160864000	0.362738000
C	0.594687000	1.608614000	2.563849000
H	-0.360518000	1.879845000	3.016101000
H	1.375277000	1.992510000	3.223824000
H	0.657020000	0.518247000	2.590444000
C	0.371924000	3.719604000	1.312468000
H	0.554533000	4.291263000	0.404124000
H	0.982932000	4.168113000	2.099543000
H	-0.669784000	3.857977000	1.604515000
C	-0.752459000	2.224523000	-1.521678000
C	-1.439456000	1.311545000	-2.537334000
H	-0.784943000	0.517096000	-2.885674000
H	-1.738793000	1.912414000	-3.399066000
H	-2.335671000	0.841227000	-2.132356000
C	-1.703627000	3.390418000	-1.241896000
H	-2.675187000	3.050671000	-0.884171000
H	-1.883143000	3.926640000	-2.176084000
H	-1.315529000	4.110648000	-0.528837000
C	0.539368000	2.749341000	-2.146497000
H	0.993834000	3.541792000	-1.554658000
H	0.319077000	3.168842000	-3.130070000
H	1.277497000	1.959887000	-2.288051000
H	0.926959000	-3.461091000	0.261034000
C	-0.708661000	-4.154443000	-0.765441000
C	-0.343841000	-5.601503000	-0.440577000

H	0.738387000	-5.743239000	-0.469081000
H	-0.784008000	-6.277492000	-1.172534000
H	-0.699122000	-5.914242000	0.540448000
C	-0.166823000	-3.803142000	-2.141582000
H	-0.493619000	-2.811044000	-2.445537000
H	-0.518128000	-4.526664000	-2.876765000
H	0.924153000	-3.819921000	-2.156098000
C	-2.213315000	-3.946646000	-0.732847000
H	-2.656272000	-4.269749000	0.209569000
H	-2.684079000	-4.523024000	-1.527891000
H	-2.450488000	-2.893435000	-0.886600000
C	1.152084000	-0.809944000	-1.637893000
H	-3.894356000	-1.457884000	4.258515000
H	-1.207497000	-0.979844000	-1.077104000
H	-2.711587000	1.097651000	0.134385000
O	0.934441000	-1.571693000	3.530170000
C	2.072291000	-1.825576000	3.085556000
C	2.585877000	-3.274171000	3.124021000
H	2.214583000	-3.835078000	2.261445000
H	2.103766000	-3.724380000	3.996324000
C	4.089125000	-3.422785000	3.238532000
H	4.378360000	-4.456688000	3.425745000
H	4.609478000	-3.098891000	2.338185000
H	4.474124000	-2.821483000	4.063316000
N	2.032205000	-1.293834000	1.207946000
C	3.303231000	-1.455978000	0.500395000
H	3.459122000	-0.651256000	-0.231815000
H	4.140383000	-1.362077000	1.209483000
C	3.410766000	-2.777886000	-0.228685000
H	2.654054000	-2.853931000	-1.012125000
H	3.287330000	-3.626781000	0.446435000

H	4.381599000	-2.889002000	-0.710922000
H	2.912354000	-1.107827000	3.276109000
H	2.042054000	-0.333474000	1.529100000
Symmetry	A		
Frequency	-213.7634		
Red. masses	7.6414		
Frc consts	0.2057		
IR Inten	138.9783		
Symmetry	A		
Frequency	27.7949		
Red. masses	4.2413		
Frc consts	0.0019		
IR Inten	0.6938		

TS3D1

N	-1.279277000	0.950211000	-0.000798000
H	-0.502796000	2.157324000	-1.384278000
C	-1.277543000	1.681658000	1.123240000
O	-0.260234000	2.313867000	1.489250000
N	1.291060000	1.109223000	-0.352282000
C	1.343609000	1.718647000	-1.713636000
H	1.262109000	0.864606000	-2.410069000
O	0.267880000	2.582603000	-1.821583000
H	0.232526000	0.743926000	-0.266095000
H	1.187967000	1.850576000	0.368640000
C	2.296577000	0.099339000	0.002208000
H	2.325836000	-0.634329000	-0.806493000
H	3.281291000	0.567995000	0.042559000
C	1.942551000	-0.544308000	1.321975000
H	0.971012000	-1.034275000	1.271409000
H	1.892847000	0.197881000	2.117250000

H	2.686003000	-1.288999000	1.596322000
C	-2.407518000	0.111063000	-0.342569000
H	-3.360871000	0.542626000	-0.018591000
H	-2.474573000	0.054893000	-1.433962000
C	-2.275546000	-1.298286000	0.209952000
H	-2.223141000	-1.289631000	1.299737000
H	-1.361992000	-1.770746000	-0.155227000
H	-3.114873000	-1.931119000	-0.079855000
C	-2.526898000	1.781224000	1.988801000
H	-3.334796000	2.199699000	1.381109000
H	-2.865503000	0.772832000	2.243217000
C	-2.322502000	2.606210000	3.238281000
H	-2.012201000	3.619219000	2.991667000
H	-1.538199000	2.183633000	3.863481000
H	-3.237026000	2.660812000	3.828152000
C	2.626302000	2.473531000	-1.972842000
H	2.731792000	3.235086000	-1.195481000
H	3.469335000	1.787354000	-1.865219000
C	2.641240000	3.111321000	-3.346412000
H	1.822512000	3.819135000	-3.453207000
H	2.534520000	2.361915000	-4.131276000
H	3.574093000	3.642516000	-3.523232000

Symmetry A

Frequency -142.1053

Red. masses 3.1678

Frc consts 0.0377

IR Inten 111.5732

Symmetry A

Frequency 28.8718

Red. masses 3.4084

Frc consts 0.0017

IR Inten 0.3846

TS3D2

N	1.645687000	-0.209902000	-0.226305000
H	0.901336000	1.024658000	-0.051464000
C	1.070549000	-1.260934000	-0.760730000
O	-0.167885000	-1.288108000	-1.053407000
N	-1.658493000	0.741974000	-0.511565000
C	-0.892121000	1.446109000	0.634720000
H	-0.754880000	0.623873000	1.360041000
O	0.257833000	1.899159000	0.107545000
H	-0.980037000	-0.072378000	-0.814758000
H	-1.716556000	1.411224000	-1.275773000
C	1.873756000	-2.511808000	-1.055574000
H	2.711681000	-2.233708000	-1.702509000
H	2.350313000	-2.838545000	-0.126024000
C	1.070392000	-3.634450000	-1.669680000
H	0.619592000	-3.326045000	-2.610983000
H	0.255033000	-3.937974000	-1.015743000
H	1.694829000	-4.506518000	-1.861225000
C	3.058952000	-0.232566000	0.083625000
H	3.303700000	-1.059729000	0.764919000
H	3.661899000	-0.414960000	-0.817544000
C	3.487852000	1.074472000	0.713050000
H	2.934769000	1.265162000	1.632646000
H	3.297611000	1.913206000	0.043737000
H	4.550254000	1.066926000	0.952262000
C	-2.977128000	0.155863000	-0.202109000
H	-2.837302000	-0.451854000	0.693172000
H	-3.672604000	0.956217000	0.054678000
C	-3.484836000	-0.680308000	-1.351306000
H	-2.780852000	-1.475008000	-1.591459000

H	-3.632786000	-0.076236000	-2.246584000
H	-4.441540000	-1.132380000	-1.099065000
C	-1.727740000	2.556581000	1.240904000
H	-2.623160000	2.140617000	1.709307000
H	-1.129090000	2.972286000	2.052066000
C	-2.086062000	3.645622000	0.249915000
H	-2.776706000	3.291278000	-0.519251000
H	-1.192985000	4.016970000	-0.249770000
H	-2.572965000	4.485737000	0.740694000

Symmetry A

Frequency -284.9471

Red. masses 2.4625

Frc consts 0.1178

IR Inten 386.7087

Symmetry A

Frequency 21.5144

Red. masses 3.3657

Frc consts 0.0009

IR Inten 0.8899

TS4

Ru	0.074761000	-0.970452000	-0.361009000
P	-0.393961000	1.199357000	0.127954000
N	0.229462000	-3.130799000	-0.154070000
O	1.526301000	-0.188484000	-2.859566000
C	-1.935258000	-1.778822000	3.975358000
N	-1.015804000	-1.303847000	1.439090000
C	-1.736687000	0.990504000	1.391929000
H	-1.838179000	1.841747000	2.067256000
C	-1.589501000	-0.298094000	2.133126000
C	-2.052658000	-0.510687000	3.416537000

H	-2.494930000	0.305954000	3.970909000
C	-1.416623000	-2.811336000	3.222898000
H	-1.321150000	-3.810985000	3.622632000
C	-0.983967000	-2.549882000	1.927832000
C	-0.547455000	-3.607227000	0.975343000
H	-1.491194000	-4.095994000	0.665540000
H	-0.029326000	-4.384618000	1.562333000
C	0.906239000	2.188005000	1.099508000
C	2.235764000	2.115247000	0.349323000
H	3.013410000	2.607992000	0.937275000
H	2.196046000	2.608254000	-0.620773000
H	2.543130000	1.084160000	0.185524000
C	1.059695000	1.476708000	2.447284000
H	0.213948000	1.666560000	3.108702000
H	1.952235000	1.850755000	2.953047000
H	1.171917000	0.398240000	2.347424000
C	0.560466000	3.644235000	1.388934000
H	0.538219000	4.263625000	0.494515000
H	1.323592000	4.064716000	2.048645000
H	-0.395496000	3.749492000	1.903367000
C	-1.206386000	2.330786000	-1.153409000
C	-2.086051000	1.453785000	-2.045814000
H	-1.499296000	0.731345000	-2.607833000
H	-2.618482000	2.092421000	-2.754265000
H	-2.831716000	0.896108000	-1.477807000
C	-2.096889000	3.418805000	-0.552457000
H	-2.919197000	3.002078000	0.028769000
H	-2.546630000	3.994212000	-1.364708000
H	-1.561357000	4.121541000	0.078075000
C	-0.128177000	2.962748000	-2.032288000
H	0.466202000	3.703335000	-1.500109000

H	-0.602275000	3.474789000	-2.872402000
H	0.547793000	2.215256000	-2.447092000
K	2.699511000	-3.474557000	0.995719000
C	0.139086000	-4.066339000	-1.294754000
C	0.392632000	-5.515008000	-0.845346000
H	1.352894000	-5.620966000	-0.332360000
H	0.418275000	-6.182584000	-1.706465000
H	-0.379270000	-5.887229000	-0.173430000
C	1.210523000	-3.715139000	-2.320295000
H	1.014484000	-2.758592000	-2.794952000
H	1.253661000	-4.470228000	-3.105930000
H	2.203377000	-3.658034000	-1.866275000
C	-1.223622000	-4.013438000	-1.994420000
H	-2.037914000	-4.249605000	-1.307907000
H	-1.278828000	-4.726579000	-2.819243000
H	-1.398692000	-3.013063000	-2.387567000
C	0.977367000	-0.535820000	-1.890654000
H	-2.265846000	-1.955977000	4.990619000
H	-1.269805000	-1.051271000	-1.189319000
H	-2.667670000	0.936379000	0.818322000
H	1.913803000	-0.973860000	0.614612000
H	2.323573000	-1.064504000	1.320426000
C	3.294937000	-1.336146000	2.962614000
S	2.071578000	-2.031244000	3.945195000
O	1.744528000	-3.402296000	3.367308000
C	2.889266000	-2.485298000	5.498244000
H	4.263833000	-1.833923000	3.078050000
H	3.375153000	-0.268823000	3.156056000
H	3.234946000	-1.584768000	6.001316000
H	2.183369000	-3.019697000	6.131614000
H	3.733771000	-3.131906000	5.262456000

Symmetry A
 Frequency -28.3856
 Red. masses 3.8160
 Frc consts 0.0018
 IR Inten 10.0749
 Symmetry A
 Frequency 31.0470
 Red. masses 2.8389
 Frc consts 0.0016
 IR Inten 4.0007

TS5

Ru	-0.297656000	-1.156513000	-0.433783000
P	-0.172513000	1.122890000	-0.091562000
N	-1.051477000	-3.195306000	-0.280681000
O	1.328152000	-1.373323000	-2.942734000
C	-2.791502000	-1.088642000	3.750710000
N	-1.478354000	-1.044588000	1.343082000
C	-1.632528000	1.340622000	1.055481000
H	-1.584339000	2.255313000	1.667675000
C	-1.878085000	0.119617000	1.887154000
C	-2.532805000	0.127803000	3.118038000
H	-2.845849000	1.073751000	3.563960000
C	-2.408722000	-2.280003000	3.142202000
H	-2.615548000	-3.246049000	3.608945000
C	-1.742854000	-2.230672000	1.915708000
C	-1.227690000	-3.414895000	1.143851000
H	-1.860499000	-4.290288000	1.386786000
H	-0.242025000	-3.660418000	1.584119000
C	1.258115000	1.850421000	0.942883000
C	2.570916000	1.493624000	0.245729000

H	3.415389000	1.602082000	0.946204000
H	2.780480000	2.140138000	-0.616697000
H	2.561960000	0.454843000	-0.113492000
C	1.165133000	1.105609000	2.276880000
H	0.349763000	1.491810000	2.907838000
H	2.095770000	1.215300000	2.855414000
H	0.991143000	0.027546000	2.139284000
C	1.214963000	3.348030000	1.222351000
H	1.384081000	3.960154000	0.325389000
H	2.015194000	3.605606000	1.935957000
H	0.269039000	3.668535000	1.685269000
C	-0.588260000	2.328298000	-1.507557000
C	-1.572073000	1.644911000	-2.457410000
H	-1.140570000	0.752894000	-2.928924000
H	-1.855003000	2.353872000	-3.252610000
H	-2.496875000	1.326714000	-1.953658000
C	-1.230181000	3.630111000	-1.024748000
H	-2.207164000	3.460786000	-0.549423000
H	-1.414757000	4.287408000	-1.889946000
H	-0.609188000	4.196100000	-0.321196000
C	0.692000000	2.630499000	-2.285745000
H	1.381954000	3.279539000	-1.729299000
H	0.442568000	3.156984000	-3.220728000
H	1.232483000	1.712709000	-2.563897000
K	1.387197000	-4.018326000	-1.073191000
C	-2.211406000	-3.622773000	-1.087533000
C	-2.374160000	-5.150946000	-1.000887000
H	-1.465175000	-5.663784000	-1.356629000
H	-3.213121000	-5.501168000	-1.621804000
H	-2.569792000	-5.503929000	0.021690000
C	-1.950084000	-3.293088000	-2.555618000

H	-1.916695000	-2.209848000	-2.728732000
H	-2.730349000	-3.724188000	-3.200972000
H	-0.984568000	-3.707191000	-2.893004000
C	-3.530310000	-2.966077000	-0.658549000
H	-3.801283000	-3.237910000	0.374356000
H	-4.371759000	-3.272249000	-1.300558000
H	-3.443921000	-1.869870000	-0.706889000
C	0.683762000	-1.249769000	-1.958902000
H	-3.306191000	-1.102973000	4.714767000
H	-1.626001000	-0.753666000	-1.249414000
H	-2.503825000	1.462810000	0.387157000
O	2.016621000	-3.824713000	1.347001000
C	2.000453000	-2.589468000	1.672214000
H	1.126692000	-1.880568000	0.742370000
C	3.271060000	-1.777942000	1.371946000
H	4.047317000	-2.165081000	2.057279000
H	3.124930000	-0.722140000	1.646773000
C	3.765527000	-1.919688000	-0.045835000
H	4.654531000	-1.303360000	-0.238502000
H	4.043404000	-2.963677000	-0.261805000
H	2.997150000	-1.603168000	-0.770707000
N	1.457014000	-2.259300000	2.946905000
H	1.888026000	-1.452115000	3.395381000
C	1.075643000	-3.292629000	3.877009000
H	0.233533000	-3.883432000	3.475918000
H	1.880128000	-4.045794000	4.025280000
C	0.683849000	-2.671516000	5.198947000
H	-0.172507000	-1.991895000	5.075515000
H	1.505081000	-2.065351000	5.612094000
H	0.410778000	-3.434355000	5.941297000
C	4.443141000	-2.726713000	4.813132000

S	4.625571000	-0.947590000	4.496476000
O	3.237296000	-0.348181000	4.538780000
C	5.369175000	-0.530772000	6.097429000
H	3.904679000	-3.155271000	3.958169000
H	5.434129000	-3.191899000	4.897352000
H	3.859043000	-2.878213000	5.730690000
H	6.348167000	-1.014496000	6.207594000
H	5.489482000	0.558381000	6.115605000
H	4.683006000	-0.837721000	6.897368000

Symmetry A

Frequency -715.5239

Red. masses 1.7038

Frc consts 0.5139

IR Inten 3114.8884

Symmetry A

Frequency 21.1141

Red. masses 4.8126

Frc consts 0.0013

IR Inten 1.3062

TS6

Ru	0.292168000	-0.978261000	-0.128183000
P	-0.288140000	1.251024000	-0.139655000
N	0.052757000	-3.117335000	0.213800000
O	1.831900000	-0.921361000	-2.691127000
C	-2.739171000	-1.265000000	3.675530000
N	-1.025711000	-1.017897000	1.555453000
C	-1.801666000	1.174472000	0.945002000
H	-2.020409000	2.114530000	1.453801000
C	-1.808102000	0.017781000	1.888189000
C	-2.659330000	-0.069523000	2.979499000

H	-3.276948000	0.776220000	3.249698000
C	-1.972568000	-2.344616000	3.269768000
H	-2.052087000	-3.305284000	3.763266000
C	-1.103232000	-2.189779000	2.200408000
C	-0.181645000	-3.236250000	1.643836000
H	-0.544007000	-4.226154000	1.947943000
H	0.774947000	-3.105212000	2.166014000
C	0.729832000	2.620898000	0.710167000
C	2.062630000	2.822393000	-0.030197000
H	2.860779000	3.038654000	0.682045000
H	2.013191000	3.662316000	-0.720086000
H	2.368738000	1.950429000	-0.607966000
C	0.976898000	2.061626000	2.114089000
H	0.065806000	2.041220000	2.713372000
H	1.699600000	2.688206000	2.641584000
H	1.363044000	1.045530000	2.098362000
C	0.063447000	3.984649000	0.867423000
H	-0.038605000	4.511945000	-0.079547000
H	0.687406000	4.610771000	1.510757000
H	-0.918071000	3.929338000	1.339519000
C	-1.015672000	1.995745000	-1.734422000
C	-1.647560000	0.891089000	-2.580649000
H	-0.916973000	0.160316000	-2.919439000
H	-2.106020000	1.348141000	-3.461129000
H	-2.428814000	0.351107000	-2.044600000
C	-2.105119000	3.041459000	-1.481455000
H	-3.003989000	2.602038000	-1.050607000
H	-2.399908000	3.478873000	-2.437928000
H	-1.791978000	3.857429000	-0.838195000
C	0.109503000	2.626459000	-2.552296000
H	0.475410000	3.549518000	-2.107581000

H	-0.263846000	2.874805000	-3.547880000
H	0.953702000	1.948484000	-2.680942000
K	2.631137000	-3.394369000	-0.481925000
C	-0.902158000	-3.904264000	-0.592695000
C	-0.667334000	-5.404546000	-0.352080000
H	0.361012000	-5.678632000	-0.596060000
H	-1.329107000	-6.009674000	-0.973662000
H	-0.846735000	-5.696718000	0.681769000
C	-0.634854000	-3.649036000	-2.072668000
H	-0.876283000	-2.626343000	-2.354096000
H	-1.226883000	-4.324937000	-2.691024000
H	0.415065000	-3.818798000	-2.323298000
C	-2.376161000	-3.592638000	-0.304659000
H	-2.649775000	-3.855830000	0.718917000
H	-3.039431000	-4.152802000	-0.966882000
H	-2.574803000	-2.528934000	-0.446652000
C	1.254879000	-0.933293000	-1.669746000
H	-3.417183000	-1.359331000	4.514525000
H	-1.036620000	-1.024823000	-0.976292000
H	-2.632555000	1.008515000	0.251910000
O	3.517242000	-3.730355000	1.790634000
C	3.257278000	-2.744673000	2.520846000
C	4.407187000	-2.037423000	3.218870000
H	5.078347000	-1.598103000	2.479912000
H	4.989875000	-2.839233000	3.681181000
C	3.999238000	-1.027076000	4.270022000
H	4.850085000	-0.453824000	4.637984000
H	3.250304000	-0.323794000	3.901571000
H	3.558853000	-1.529508000	5.133485000
N	2.379612000	-1.271568000	1.451254000
C	3.382893000	-0.286849000	1.055003000

H	2.901171000	0.610259000	0.669093000
H	3.990126000	0.064929000	1.902099000
C	4.319545000	-0.817055000	-0.011866000
H	3.797273000	-0.977475000	-0.957508000
H	4.785973000	-1.755205000	0.299353000
H	5.122236000	-0.109788000	-0.219383000
H	2.356561000	-2.780059000	3.178390000
H	1.862434000	-0.874232000	2.237166000
C	1.213434000	-0.101571000	6.765233000
S	0.107177000	-0.803367000	5.524077000
O	0.588719000	-0.326525000	4.203420000
C	0.663206000	-2.509035000	5.709854000
H	1.045639000	0.972005000	6.775619000
H	0.980439000	-0.516496000	7.743761000
H	2.245684000	-0.310149000	6.491756000
H	0.383050000	-2.883350000	6.692602000
H	0.165561000	-3.091332000	4.938010000
H	1.740000000	-2.564663000	5.563182000

Symmetry A

Frequency -235.9341

Red. masses 7.8358

Frc consts 0.2570

IR Inten 235.0520

Symmetry A

Frequency 23.8028

Red. masses 4.0787

Frc consts 0.0014

IR Inten 2.1194

TS7

Ru	0.149274000	-0.987047000	-0.274872000
----	-------------	--------------	--------------

P	-0.194266000	1.203666000	0.123531000
N	-0.002177000	-3.280012000	0.104256000
O	2.477482000	-0.692290000	-2.127796000
C	-3.219369000	-1.413737000	3.205752000
N	-1.343293000	-1.164272000	1.231689000
C	-1.915496000	1.088073000	0.714481000
H	-2.358314000	1.993280000	1.131661000
C	-2.103538000	-0.078224000	1.537327000
C	-3.044341000	-0.201802000	2.577634000
H	-3.623721000	0.663369000	2.872509000
C	-2.443513000	-2.514606000	2.842798000
H	-2.554920000	-3.472717000	3.331099000
C	-1.484912000	-2.332235000	1.863183000
C	-0.455531000	-3.364204000	1.509177000
H	0.418947000	-3.163984000	2.134533000
H	-2.856937000	0.648889000	-0.379103000
C	0.727125000	1.965853000	1.612587000
C	2.233961000	2.009342000	1.363737000
H	2.750551000	2.214177000	2.304177000
H	2.532772000	2.782307000	0.662769000
H	2.595208000	1.049260000	0.992412000
C	0.494975000	1.048438000	2.817561000
H	-0.541506000	1.055144000	3.149726000
H	1.102870000	1.409672000	3.649834000
H	0.786622000	0.020079000	2.609065000
C	0.181860000	3.340619000	1.995618000
H	0.335359000	4.103727000	1.237655000
H	0.680285000	3.688211000	2.903768000
H	-0.885500000	3.296597000	2.215665000
C	-0.141491000	2.442575000	-1.336301000
C	0.035349000	1.646850000	-2.639781000

H	1.090484000	1.456476000	-2.826840000
H	-0.346511000	2.231367000	-3.480288000
H	-0.447253000	0.675360000	-2.631318000
C	-1.440644000	3.245796000	-1.368668000
H	-2.311014000	2.610338000	-1.527325000
H	-1.405060000	3.966080000	-2.189198000
H	-1.602994000	3.805668000	-0.446432000
C	1.035955000	3.417335000	-1.313018000
H	1.026730000	4.120153000	-0.484859000
H	1.000220000	4.006578000	-2.232484000
H	1.989175000	2.892139000	-1.315359000
H	0.990470000	-3.486058000	0.096820000
C	-0.641349000	-4.258991000	-0.842346000
C	-0.210773000	-5.681361000	-0.492629000
H	0.873972000	-5.789757000	-0.545998000
H	-0.645528000	-6.389432000	-1.197440000
H	-0.533932000	-5.982619000	0.503994000
C	-0.139816000	-3.896655000	-2.230899000
H	-0.461134000	-2.888398000	-2.489826000
H	-0.530974000	-4.596906000	-2.969386000
H	0.950227000	-3.940365000	-2.277402000
C	-2.152101000	-4.119436000	-0.763413000
H	-2.541949000	-4.418629000	0.211364000
H	-2.618461000	-4.762632000	-1.509870000
H	-2.430533000	-3.086147000	-0.969465000
C	1.544695000	-0.807852000	-1.439567000
H	-3.954138000	-1.509218000	3.995815000
H	1.282666000	-1.072514000	0.851762000
O	-1.672851000	-1.165748000	-1.702567000
C	-2.602985000	-0.428710000	-2.272556000
C	-3.341647000	-1.159710000	-3.395936000

H	-4.233819000	-0.598182000	-3.696586000
H	-3.681217000	-2.129710000	-3.022998000
C	-2.423129000	-1.360006000	-4.583521000
H	-2.912990000	-1.898674000	-5.393291000
H	-2.080859000	-0.403243000	-4.981797000
H	-1.538847000	-1.923051000	-4.288439000
N	-3.619202000	0.104764000	-1.216274000
C	-4.456054000	-0.908804000	-0.558669000
H	-4.891116000	-1.571642000	-1.310863000
H	-3.794428000	-1.523033000	0.052934000
C	-5.544045000	-0.268465000	0.268570000
H	-6.256446000	0.268064000	-0.359891000
H	-5.131788000	0.440152000	0.985761000
H	-6.098988000	-1.018967000	0.828572000
H	-2.271288000	0.546338000	-2.695605000
H	-4.213811000	0.804490000	-1.654584000
H	-0.809540000	-4.364209000	1.773941000

Symmetry A

Frequency -1200.2262

Red. masses 1.1184

Frc consts 0.9492

IR Inten 3291.3404

Symmetry A

Frequency 32.9655

Red. masses 3.4451

Frc consts 0.0022

IR Inten 0.1425